# **EAST Search History**

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	2544	((544/330,332) or (514/275)).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2006/11/21 23:01

11/21/2006 11:01:30 PM Page 1

	NPL Search Notes	Results
6.	TITLE-ABSTR-KEY(IgE-mediated or immunoglobulin synthesis) and TITLE-ABSTR-KEY (transplant rejection) [All Sources(- All Sciences -)]	2
5.	TITLE-ABSTR-KEY(IgE-mediated or immunoglobulin synthesis) and TITLE-ABSTR-KEY (gastrointestinal) [All Sources(- All Sciences -)]	172
4.	TITLE-ABSTR-KEY(IgE-mediated or immunoglobulin synthesis) and TITLE-ABSTR-KEY (autoimmune) [All Sources(- All Sciences -)]	81
3.	(TITLE-ABSTR-KEY(IgE-mediated)) AND (TITLE-ABSTR-KEY(immunoglobulin synthesis)) [All Sources(- All Sciences -)]	1
2.	TITLE-ABSTR-KEY(IgE-mediated) [All Sources(- All Sciences -)]	4083
1.	TITLE-ABSTR-KEY(immunoglobulin synthesis) [All Sources(- All Sciences -)]	1304

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C:\Program Files\Stnexp\Queries\10501445.str

chain nodes:

19 22 23 26

ring nodes:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

chain bonds:

5-19 9-19 22-23

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds:

5-19 9-19 22-23

normalized bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18

isolated ring systems:

containing 1: 7: 13:

G1:Cl,Br,F,I,X,[\*1]

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLAS\$20:Atom 22:CLAS\$23:CLAS\$26:CLAS\$27:Atom

Generic attributes:

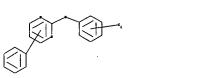
22:

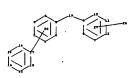
Saturation : Saturated

Number of Carbon Atoms: less than 7

=>

Uploading C:\Program Files\Stnexp\Queries\10501445.str





```
chain nodes :
19 22 23 26
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
5-19 9-19 22-23
ring bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-12 \quad 8-9 \quad 9-10 \quad 10-11 \quad 11-12 \quad 13-14 \quad 13-18
14-15 15-16 16-17 17-18
exact/norm bonds :
5-19 9-19 22-23
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-12 \quad 8-9 \quad 9-10 \quad 10-11 \quad 11-12 \quad 13-14 \quad 13-18
14-15 15-16 16-17 17-18
isolated ring systems:
containing 1:7:13:
```

## G1:C1,Br,F,I,X,[\*1]

## Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:Atom 22:CLASS 23:CLASS 26:CLASS 27:Atom Generic attributes : 22:

Saturation : Saturated Number of Carbon Atoms : less than 7

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 17:11:14 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2235 TO ITERATE

89.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

41865 TO 47535

PROJECTED ANSWERS:

11 TO

9 ANSWERS

378 ANSWERS

9 SEA SSS SAM L1

=> => s l1 sss ful

FULL SEARCH INITIATED 17:12:43 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 46908 TO ITERATE

100.0% PROCESSED 46908 ITERATIONS

SEARCH TIME: 00.00.03

378 SEA SSS FUL L1

=> => s 13

47 L3 · L4

=> d 14 1-47 bib, ab, hitstr

```
ANSWER 1 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
     2006:542661 CAPLUS
AN
DN
     145:46082
ΤI
     Preparation of substituted heterocycles for treating HGF mediated diseases
IN
     Kim, Tae-Seong; Bellon, Steven; Booker, Shon; D'Angelo, Noel; Dominguez,
     Celia; Fellows, Ingrid; Lee, Matthew; Liu, Longbin; Rainbeau, Elizabeth;
     Siegmund, Aaron C.; Tasker, Andrew; Xi, Ning; Cheng, Yuan
PA
     Amgen Inc., USA
     PCT Int. Appl., 228 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                             APPLICATION NO.
                                                                     DATE
                                 20060608
PΙ
     WO 2006060318
                          A2
                                             WO 2005-US42935
                                                                     20051129
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                          A3
                                 20060720
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
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             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
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             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     US 2006252777
                          A1
                                 20061109
                                             US 2005-289659
                                                                      20051129
PRAI US 2004-632271P
                           Ρ
                                 20041130
     MARPAT 145:46082
OS
AΒ
     The title compds. RIXWAYR [I; R = (un)substituted aryl, heterocyclyl,
     cycloalkyl, etc.; R1 = II (wherein ring T = Ph, 5-6 membered heteroaryl; Z
     = N or CH; R10 = alkoxy, haloalkoxy, arylalkoxy, etc.); W =
     (un) substituted aryl, 5-6 membered heteroaryl; A = (un) substituted 5-7
     membered N-containing heterocyclyl; X = O, S, NR2, CR3R4; Y = a bond, CO,
     CONH, etc.; R2 = H, alkyl, haloalkyl, etc.; R3, R4 = H, alkyl, aryl, etc.]
     which are effective for prophylaxis and treatment of diseases, such as HGF
     mediated diseases, were prepared E.g., a multi-step synthesis of III,
     starting from 2-benzyl-3H-pyrimidin-4-one, was given. Compds. I showed
     inhibition of c-Met kinase at doses less than 2 μM. The invention
     encompasses novel compds. I, analogs, prodrugs and pharmaceutically
     acceptable salts thereof, pharmaceutical compns. and methods for
     prophylaxis and treatment of diseases and other maladies or conditions
     involving, cancer and the like. The subject invention also relates to
     processes for making such compds. as well as to intermediates useful in
     such processes.
ΙT
     890020-03-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
         (preparation of substituted heterocycles for treating HGF mediated diseases)
RN
     890020-03-8 CAPLUS
     4(1H)-Pyrimidinone, 5-[4-[(6,7-dimethoxy-4-quinolinyl)oxy]-3-fluorophenyl]-
CN
```

2-[(4-fluoro-2-methylphenyl)amino]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

Page 4

```
T.4
    ANSWER 2 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
AN
    2006:440209 CAPLUS
DN
    144:468191
     Preparation of phenylpyrimidinecarboxamides as modulators of voltage-gated
ΤI
    sodium and calcium channels
    Martinborough, Esther; Zimmermann, Nicole; Perni, Robert; Arnost, Michael;
IN
    Bandarage, Upul; Maltais, Francois; Bemis, Guy
    Vertex Pharmaceuticals Incorporated, USA
PA
    PCT Int. Appl., 166 pp.
SO
    CODEN: PIXXD2
DТ
    Patent
    English
LΑ
FAN.CNT 1
    PATENT NO.
                         KIND
                                `DATE
                                            APPLICATION NO.
                                                                    DATE
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                         ____
                                            ______
PΙ
    WO 2006050476
                          A2
                                20060511
                                            WO 2005-US39881
                                                                    20051103
    WO 2006050476
                          A3
                                2006101/9
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
    US 2006160817
                                20060720
                          A1
                                            US 2005-266142
                                                                    20051103
PRAI US 2004-624716P
                          Ρ
                                20041103
    US 2004-624718P
                          ₽
                                20041103
    US 2004-624800P
                          Ρ
                                20041103
OS.
    MARPAT 144:468191
    Title compds. I [wherein X = halo, cyano, Me, etc.; n = 1-4; R1, R2 = H,
AΒ
     alkyl, cycloalkyl, etc.; R3, R4 = H, alkyl, heterocyclyl, etc.; Y = H or
    alkyl] and pharmaceutically acceptable salts thereof were prepared as ion
     channel modulators, especially as voltage-gated sodium and calcium channel
     inhibitors. For instance, II was synthesized in multiple steps and showed
     inhibitory activity for CaV 2.2, Nav 1.3 and NaV 1.8 with IC50 values of <
     10.0~\mu\text{M}. I and their pharmaceutical compns. are useful for the
     treatment of various diseases.
ΙT
     886196-10-7P 886196-14-1P 886196-39-0P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (inhibitor; preparation of phenylpyrimidinecarboxamides as inhibitors of
        voltage-gated sodium and calcium channels)
RN
     886196-10-7 CAPLUS
CN
     5-Pyrimidinecarboxamide, 2-[(3-chlorophenyl)amino]-4-(2-fluorophenyl)-N-(1-
    methylethyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)
```

RN 886196-14-1 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-fluorophenyl)-2-[(4-fluorophenyl)amino]-N-(1-methylethyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 886196-39-0 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[(4-chlorophenyl)amino]-4-(2-fluorophenyl)-N-(1-methylethyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

```
L4
     ANSWER 3 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
     2006:340006 CAPLUS
ΑN
     144:390933
DN
ΤI
     Preparation of anilinopyrimidines as IKK kinase inhibitors
     Sum, Fuk-Wah; Powell, Dennis William; Zhang, Yixian; Chen, Lijing;
IN
     Kincaid, Scott Lee; Jennings, Lee Dalton; Hu, Yongbo; Gilbert, Adam
     Matthew; Bursavich, Matthew Gregory
     Wyeth, John, and Brother Ltd., USA
PA
so
     U.S. Pat. Appl. Publ., 55 pp.
     CODEN: USXXCO
DT
     Patent
     English
LΑ
FAN.CNT 1
     PATENT NO.
                         KIND
                                  ATE
                                             APPLICATION NO.
                                                                     DATE
                                             -----
                                 20060413
PΤ
     US 2006079543
                          A1
                                             US 2005-248495
                                                                     20051013
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                                             WO 2005-US36674
                                                                     20051013
             AE, AG, AL, AM, AT,
                                 AU, AZ
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,
             NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,
             YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRAI US 2004-617668P
                          Ρ
                                 20041013
OS
     MARPAT 144:390933
AB
     Title compds. I [wherein R1, R4 = H; R2 = (un) substituted amino,
     guanidinyl, ureido, etc.; R3 = H, (un)substituted Ph, certain heteroaryl,
     etc.; R5 = H, alkyl, alkylsulfonyl, etc.; R6 = H, halo, (un)substituted
     Ph, etc.] and salts, solvates or hydrates thereof were prepared as kinase
     inhibitors, especially IKK kinase inhibitors. For instance, condensation of
     2-acetyl-5-chlorothiophene with DMF di-Me acetal followed by cyclization
     with a guanidine, which was obtained by treatment of sulfanilamide with
     1H-pyrazole-1-carboximidamide hydrochloride, gave 2-pyrimidinamine II.
     Exemplary I gave a pos. or slightly pos. result in the western anal. of
           Therefore, I and their pharmaceutical compns. are useful for
     the treatment of diseases associated with NF-kB activation, such as
     inflammation, tumor and ischemic conditions.
     882875-57-2P 882875-63-0P 882875-64-1P
     882875-65-2P 882875-66-3P 882875-68-5P
     882875-69-6P 882875-70-9P 882875-71-0P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (drug candidate; preparation of anilinopyrimidines as IKK kinase inhibitors)
RN
     882875-57-2 CAPLUS
CN
     Benzenesulfonamide, 2-chloro-5-[[4-(3-fluoro-4-methoxyphenyl)-2-
     pyrimidinyl]amino]- (9CI) (CA INDEX NAME)
```

RN 882875-63-0 CAPLUS

CN Benzenesulfonamide, N-[3-(dimethylamino)propyl]-4-[[4-(3-fluoro-4-methoxyphenyl)-2-pyrimidinyl]amino]-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 882875-64-1 CAPLUS

CN Benzenesulfonamide, N-[2-(dimethylamino)ethyl]-4-[[4-(3-fluoro-4-methoxyphenyl)-2-pyrimidinyl]amino]-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 882875-65-2 CAPLUS

CN Benzenesulfonamide, N-[3-(dimethylamino)propyl]-4-[[4-(4-methoxyphenyl)-2-pyrimidinyl]amino]-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 882875-66-3 CAPLUS

CN Benzenesulfonamide, N-[2-(dimethylamino)ethyl]-4-[[4-(4-methoxyphenyl)-2-pyrimidinyl]amino]-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \begin{array}{c|c} \text{CF3} & \begin{array}{c} \text{O} \\ \text{S} \\ \text{NH} \end{array} \end{array} \\ \begin{array}{c|c} \text{S-NH-CH}_2 - \text{CH}_2 - \text{NMe}_2 \\ \end{array}$$

RN 882875-68-5 CAPLUS

CN Benzenesulfonamide, 2-chloro-N-[2-(dimethylamino)ethyl]-4-[[4-(3-fluoro-4-methoxyphenyl)-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

$$O = S - NH - CH_2 - CH_2 - NMe_2$$

$$C1 \qquad NH \qquad F \qquad OMe$$

RN 882875-69-6 CAPLUS

CN Benzenesulfonamide, 2-chloro-N-[2-(dimethylamino)ethyl]-4-[[4-(4-methoxyphenyl)-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \begin{array}{c|c} \text{C1} & \begin{array}{c} \text{O} \\ \text{\parallel} \\ \text{S-NH-CH}_2\text{-CH}_2\text{-NMe}_2 \end{array} \end{array}$$

RN 882875-70-9 CAPLUS

CN Benzenesulfonamide, 2-chloro-N-[3-(dimethylamino)propyl]-4-[[4-(3-fluoro-4-methoxyphenyl)-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

RN 882875-71-0 CAPLUS

CN Benzenesulfonamide, 2-chloro-N-[3-(dimethylamino)propyl]-4-[[4-(4-methoxyphenyl)-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

```
ANSWER 4 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
AN
     2006:301346 CAPLUS
DN
     144:350708
     Novel pyrimidine compounds, process for their preparation, pharmaceutical
     compositions, and their use as antiinflammatory, cytotoxic, rheumatic,
     immunosuppressive and cardiovascular agents for treatment of diseases
     Kalleda, Srinivas; Padakanti, Srinivas; Kumar Swamy, Nalivela;
IN
     Yeleswarapu, Koteswar Rao; Alexander, Christopher W.; Khanna, Ish Kumar;
     Iqbal, Javed; Pillarisetti, Sivaram; Pal, Manojit; Barange, Deepak
PA
     Reddy US Therapeutics, Inc., USA
SO
     PCT Int. Appl., 336 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LΑ
FAN.CNT 2
     PATENT NO.
                          KIND
                                  DATE
                                              APPLICATION NO.
                                                                       DATE
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     WO 2006034473
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                                              WO 2005-US34243
                                                                       20050923
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
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             YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
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             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     US 2006084644
                                 20060420
                           A1
                                              US 2005-234257
                                                                       20050923
     US 2006084645
                           A1
                                 20060420
                                              US 2005-234695
                                                                       20050923
PRAI US 2004-612374P
                           Ρ
                                 20040923
OS
     MARPAT 144:350708
AB
     The invention provides heterocyclic compds., particularly substituted
     pyrimidines of formula I, methods and compns. for making and using these
     heterocyclic compds., and methods for treating a variety of diseases and
     disease states, including atherosclerosis, arthritis, restenosis, diabetic
     nephropathy, or dyslipidemia, or disease states mediated by the low
     expression of Perlecan. Compds. of formula I wherein R1, R2 and R4 are
     independently (un) substituted (hetero) aryl or (un) substituted
     heterocyclyl; and their pharmaceutically acceptable salts, prodrugs,
     diastereoisomeric mixts., enantiomers, tautomers, and racemic mixts.
     thereof are claimed in this invention. Example compound II was prepared by
     acylation of 4-methoxyacetophenone with di-Et carbonate; the resulting Et
     4-methoxybenzoylacetate underwent cyclization with guanidine carbonate to
     give 2-amino-6-(4-methoxyphenyl)pyrimidin-4-ol, which was converted to
     4-chloro-6-(methoxyphenyl)pyrimidin-2-ylamine, which underwent amination
     with 3-chloro-4-methoxyaniline to give compound II. The invention compds.
     were evaluated for their antiinflammatory, proliferative, cardiovascular,
     and immunosuppressive activity (no data).
     881193-46-0P 881193-55-1P
IT
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
         (drug candidate; preparation of pyrimidine compds. and their use as
        antiinflammatory, proliferative, rheumatic, immunosuppressive and
        cardiovascular agents for treatment of diseases)
```

RN 881193-46-0 CAPLUS

CN 4-Piperidinol, 1-[2-[(3-chloro-4-methoxyphenyl)amino]-6-phenyl-4-pyrimidinyl]- (9CI). (CA INDEX NAME)

RN 881193-55-1 CAPLUS

CN 2-Pyrimidinamine, N-(3-fluoro-4-methoxyphenyl)-4-phenyl-6-(4-thiomorpholinyl)- (9CI) (CA INDEX NAME)

IT 881193-14-2P 881193-24-4P 881193-25-5P

881193-26-6P 881193-27-7P 881193-28-8P

881193-29-9P 881193-30-2P 881193-31-3P

881193-32-4P 881193-33-5P 881193-34-6P

881193-50-6P 881193-51-7P 881193-53-9P

881193-56-2P 881193-57-3P 881193-59-5P

881193-60-8P 881193-61-9P 881193-64-2P 881193-65-3P 881193-66-4P 881193-67-5P

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881194-24-7P 881194-27-0P 881194-29-2P

881194-30-5P 881194-31-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyrimidine compds. and their use as antiinflammatory, proliferative, rheumatic, immunosuppressive and cardiovascular agents for treatment of diseases)

RN 881193-14-2 CAPLUS

CN 2,4-Pyrimidinediamine, N,N'-bis(3-chloro-4-methoxyphenyl)-6-phenyl- (9CI) (CA INDEX NAME)

RN 881193-24-4 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chloro-4-methoxyphenyl)-N4-methyl-6-phenyl-(9CI) (CA INDEX NAME)

RN 881193-25-5 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chloro-4-methoxyphenyl)-N4-(1-methylethyl)-6-phenyl- (9CI) (CA INDEX NAME)

RN 881193-26-6 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chloro-4-methoxyphenyl)-N4-cycloheptyl-6-phenyl- (9CI) (CA INDEX NAME)

RN 881193-27-7 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chloro-4-methoxyphenyl)-6-phenyl-N4-

(phenylmethyl) - (9CI) (CA INDEX NAME)

RN 881193-28-8 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(3-chloro-4-methoxyphenyl)amino]-6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 881193-29-9 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(3-chloro-4-methoxyphenyl)amino]-6-phenyl- (9CI) (CA INDEX NAME)

RN 881193-30-2 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-ethoxy-6-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 881193-31-3 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-(4-methoxyphenyl)-6-(1-methylethoxy)- (9CI) (CA INDEX NAME)

RN 881193-32-4 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-(4-methoxyphenyl)-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 881193-33-5 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-(4-methoxyphenyl)-6-[(4-methylphenyl)methoxy]- (9CI) (CA INDEX NAME)

RN 881193-34-6 CAPLUS

CN Acetic acid, [[2-[(3-chloro-4-methoxyphenyl)amino]-6-(4-methoxyphenyl)-4-pyrimidinyl]oxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 881193-50-6 CAPLUS

CN 4-Piperidinol, 1-[2-[(3-chloro-4-hydroxyphenyl)amino]-6-phenyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 881193-51-7 CAPLUS

CN 4-Piperidinol, 1-[2-[(3-fluoro-4-methoxyphenyl)amino]-6-phenyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 881193-53-9 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-phenyl-6-(4-thiomorpholinyl)- (9CI) (CA INDEX NAME)

RN 881193-56-2 CAPLUS

CN Phenol, 2-chloro-4-[[4-phenyl-6-(4-thiomorpholinyl)-2-pyrimidinyl]amino]-(9CI) (CA INDEX NAME)

RN 881193-57-3 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-(4-morpholinyl)-6-phenyl-(9CI) (CA INDEX NAME)

RN 881193-59-5 CAPLUS

CN 2-Pyrimidinamine, N-(3-fluoro-4-methoxyphenyl)-4-(4-morpholinyl)-6-phenyl-(9CI) (CA INDEX NAME)

RN 881193-60-8 CAPLUS

CN Phenol, 2-chloro-4-[[4-(4-morpholinyl)-6-phenyl-2-pyrimidinyl]amino]-(9CI) (CA INDEX NAME)

RN 881193-61-9 CAPLUS

CN 4-Piperidinol, 1-[6-phenyl-2-[[3-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 881193-64-2 CAPLUS

CN 2-Pyrimidinamine, 4-(4-fluorophenyl)-6-(4-morpholinyl)-N-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 881193-65-3 CAPLUS

CN 2-Pyrimidinamine, N,4-bis(4-fluorophenyl)-6-(4-morpholinyl)- (9CI) (CA INDEX NAME)

RN 881193-66-4 CAPLUS

CN 4-Piperidinol, 1-[2-[[4-chloro-3-(trifluoromethyl)phenyl]amino]-6-phenyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 881193-67-5 CAPLUS

CN 2-Pyrimidinamine, 4-(4-morpholinyl)-6-phenyl-N-[3-(trifluoromethyl)phenyl]-(9CI) (CA INDEX NAME)

RN 881194-05-4 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-phenyl-6-(phenylethynyl)-(9CI) (CA INDEX NAME)

RN 881194-06-5 CAPLUS

CN Ethanol, 2-[[2-[(3-chloro-4-methoxyphenyl)amino]-6-phenyl-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

$$HO-CH_2-CH_2-NH$$
  $C1$   $N$   $NH$   $NH$ 

RN 881194-08-7 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-phenyl-6-(1-piperazinyl)-(9CI) (CA INDEX NAME)

RN 881194-24-7 CAPLUS

CN Butanedioic acid, mono[1-[2-[(3-chloro-4-methoxyphenyl)amino]-6-phenyl-4-pyrimidinyl]-4-piperidinyl] ester (9CI) (CA INDEX NAME)

RN 881194-27-0 CAPLUS

CN Cyclohexanol, 4-[[2-[(3-chloro-4-methoxyphenyl)amino]-6-phenyl-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

RN 881194-29-2 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-(4-ethyl-1-piperazinyl)-6-phenyl- (9CI) (CA INDEX NAME)

RN 881194-30-5 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-(4-methyl-1-piperazinyl)-6-phenyl- (9CI) (CA INDEX NAME)

RN 881194-31-6 CAPLUS

CN 2-Pyrimidinamine, 4-(1,1-dioxido-4-thiomorpholinyl)-N-(3-fluoro-4-methoxyphenyl)-6-phenyl- (9CI) (CA INDEX NAME)

IT 881195-06-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of pyrimidine compds. and their use as antiinflammatory, proliferative, rheumatic, immunosuppressive and cardiovascular agents for treatment of diseases)

RN 881195-06-8 CAPLUS

CN 2-Pyrimidinamine, 4-chloro-N-(3-chloro-4-methoxyphenyl)-6-phenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:180156 CAPLUS

DN 144:390868

TI Synthesis of analogs of the phenylamino-pyrimidine type protein kinase C inhibitor CGP 60474 utilizing a Negishi cross-coupling strategy

AU Stanetty, Peter; Roehrling, Juergen; Schnuerch, Michael; Mihovilovic, Marko D.

CS Institute of Applied Synthetic Chemistry, Vienna University of Technology, Vienna, A-1060, Austria

SO Tetrahedron (2006), 62(10), 2380-2387 CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier B.

DT Journal

LA English

AB Analogs of 3-[[4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-pyridinyl]amino]-1-propanol (CGP 60474) were synthesized as useful models for the evaluation of structure-activity relationships of phenylamino-pyrimidine-type protein kinase C inhibitors. The approach involved Pd-assisted cross-coupling as the key step. Negishi-type coupling was performed both with free amino functionalities and Boc-protected amines present and showed that the protection-cross-coupling-deprotection sequence leads to significantly higher yields. The results of biol. screening of the title compds. showed no improved fungicidal activity over CGP 60474 and will be reported elsewhere.

IT 883199-29-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [[[(chlorophenyl)amino]pyrimidinyl]pyridinyl]amino]propanol (CGP 60474) analogs and derivs. using (chlorophenyl)[(acylamino)phenyl] pyrimidinamine as intermediate and Negishi cross-coupling as key synthetic step)

RN 883199-29-9 CAPLUS

CN Propanoic acid, 3-[[3-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]phenyl]amino]-3-oxo-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \parallel & \parallel \\ MeO-C-CH_2-C-NH \end{array}$$

IT 883199-16-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of [[[(chlorophenyl)amino]pyrimidinyl]pyridinyl]amino]propanol (CGP 60474) analogs and derivs. using Negishi cross-coupling as key synthetic step)

RN 883199-16-4 CAPLUS

CN 1-Propanol, 3-[[3-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]phenyl]amino]-(9CI) (CA INDEX NAME)

### 10/501,445

L4ANSWER 6 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN AN 2005:1174303 CAPLUS DN 144:22887

Novel synthesis of N-phenyl-2-aminopyrimidine derivatives under ΤI solvent-free conditions.

AU

Kidemet Davor; Elenkov, Ivaylo; Prgomet, Vesna Pliva Research Institute Ltd., Zagreb, 10000, Croatia CS

Synlett (2005), (16), 2531-2533 CODEN: SYNLES; ISSN: 0936-5214 SO

Georg Thieme/Verlag PB

DTJourna N LΑ English

os CASREACT 144:22887

AΒ An efficient method for the solvent-free synthesis of N-phenyl-2aminopyrimidines was developed through cyclocondensation of N-phenylguanidine with enaminone in the presence of DBU. The procedure is exptl. simple with very short reaction times and good yields. According to this procedure a variety of N-phenyl-2-aminopyrimidines were synthesized.

İT 870002-52-1P 870002-53-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of N-phenyl-2-aminopyrimidine derivs. by cyclocondensation of N-phenylguanidine with enaminone using DBU base under solvent-free conditions)

RN 870002-52-1 CAPLUS

2-Pyrimidinamine, N-(4-fluorophenyl)-4-(2-methoxyphenyl)- (9CI) CN

RN 870002-53-2 CAPLUS

CN 2-Pyrimidinamine, N-(3-fluorophenyl)-4-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L4
     ANSWER 7 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
ΑN
     2005:1123789 CAPLUS
DN
     143:427366
     Compositions and methods for treatment of inflammatory conditions using
ΤI
     steroid sparing agents
IN
     Lieberburg, Ivan
PA
     Elan Pharmaceuticals, Inc., USA
SO
     PCT Int. Appl., 782 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
     PATENT NO.
                           KIND
                                   ÐΆΤΕ
                                                APPLICATION NO.
                                                                         DATE
PΙ
     WO 2005097162
                            A2
                                   20051020
                                                WO 2005-US11307
                                                                         20050401
     WO 2005097162
                            A3
                                   20060406
         W:
              AE, AG, AL, AM, AT
                                        AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
                                   ΑU,
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
         SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
              AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
              MR, NE, SN, TD, TG
     AU 2005231467
                            A1
                                   20051020
                                                AU 2005-231467
                                                                         20050401
     US 2006004019
                            A1
                                   20060105
                                                US 2005-95822
                                                                         20050401
PRAI US 2004-558121P
                            Ρ
                                   20040401
                                  20050401
     WO 2005-US11307
                            W
os
     MARPAT 143:427366
AΒ
     This invention relates generally to the use of a steroid sparing agent for
     the preparation of a medicament for the treatment of inflammatory bowel
     diseases (IBD), asthma, multiple sclerosis (MS), rheumatoid arthritis
     (RA), graft vs. host disease (GVHD), host vs. graft disease, and various
     spondyloarthropathies, comprising administering a steroid sparing Ig that
     modulates \alpha 4\beta 1 and \alpha 4\beta 7 integrins, or an amino
     acid-based small (heterocyclic) mol. to a patient in need thereof.
     invention also relates generally to combination therapies for the
     treatment of these conditions, including an immunosuppressant, an anti-TNF
     compound, and a 5-ASA compound For example, a steroid sparing agent was
     prepared by converting L-tyrosine tert-Bu ester to L-4-(N,N-
     dimethylcarbamyloxy)-phenylalanine tert-Bu ester and coupling it to
     4,6-dichloro-5-piperidin-1-yl-pyrimidine to give N-(5-piperidin-
     yl)pyrimidin-4-yl-L-4-(N,N-dimethylcarbamyloxy)phenylalanine. Also,
     Natalizumab, a humanized monoclonal IgG4 antibody to \alpha4 integrin,
     was evaluated in subjects with Chron's disease. Monthly administration of
     Natalizumab for 6 mo was well tolerated and enabled subjects to be
     successfully withdrawn from steroids.
TΤ
     285139-65-3P
     RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
         (preparation of steroid sparing agents for treatment of inflammatory
        conditions)
RN
     285139-65-3 CAPLUS
     L-Tyrosine, N-[2-[(4-chlorophenyl)methylamino]-5-(2-methylphenyl)-4-
CN
     pyrimidinyl]-, dimethylcarbamate (ester) (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

### 10/501,445

- L4 ANSWER 8 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2005:1024910 CAPLUS
- DN 143:381701
- TI Diamino-C,N-diarylpyridine positional isomers as inhibitors of lysophosphatidic acid acyltransferase-β
- AU Hong, Feng; Hollenback, David; Singer, Jack W.; Klein, Peter
- CS Cell Therapeutics, Inc., Seattle, WA, 98119, USA
- SO Bioorganic & Medicinal Chemistry Letters (2005) 15(21), 4703-4707 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier B.V.
- DT Journal
- LA English
- OS CASREACT 143:381701
- AB 2,6-Diamino-4,N-diarylpyridines were identified as potent, isoform selective inhibitors of the enzymic activity of lysophosphatidic acid acyltransferase- $\beta$  (LPAAT- $\beta$ ).
- IT 710334-91-1
  - RL: PAC (Pharmacological activity); BIOL (Biological study) (diamino-C,N-diarylpyridine isomers preparation and inhibition of LPAAT- $\beta$ )
- RN 710334-91-1 CAPLUS
- CN 2,4-Pýrimidinediamine, 6-(5-chloro-2-methoxyphenyl)-N2-(4-chlorophenyl)-(9CI) (CA INDEX NAME)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 9 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
AN
     2005:371231 CAPLUS
DN
     142:430290
     Preparation of 5-arylpyrimidine derivatives as inhibitors of mixed
TТ
     lymphocyte reaction
     Tsuruoka, Hiroyuki; Ueda, Kiyono; Sugano, Yuichi; Tatsuta, Toru
IN
PA
     Sankyo Company, Limited, Japan
SO
     PCT Int. Appl., 124 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     Japanese
FAN.CNT 1
     PATENT NO.
                        KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
     -----
                                            -----
                                                                   _____
     WO 2005037802
                                20050428
PΤ
                         A1
                                            WO 2004-JP15653
                                                                   20041015
         W: AE, AG, AL, AM, AR, AU, AZ,
                                        BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ÌD,—TĹ, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     JP 2005139170
                                            JP 2004-297133
                         A2
                                20050602
                                                                   20041012
PRAI JP 2003-356170
                                20031016
                         Α
     MARPAT 142:430290
OS
AΒ
     The title compds. I [R1 and R3 each is lower alkyl; R2 and R4 each is
     aryl, etc.; R5 is aryl, etc.; R6 is hydrogen; and R7 is aryl, etc.] are
     prepared Thus, 1-(4-pyridyl)-1-ethanone N-(2-anilino-5-phenyl-6-[2-[1-(4-
     pyridyl)ethylidene]hydrazono]-4-pyrimidinyl)hydrazone was prepared in 2
     steps from 4,6-dihydroxy-5-phenyl-2-phenylaminopyrimidine. Compds. of
     this invention in vitro showed IC50 values of 0.25 ng/mL to 0.53 ng/mL
     against the mixed lymphocyte reaction.
                                            Formulations are given.
IT
     850706-89-7P 850707-28-7P 850707-29-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of 5-arylpyrimidine derivs. as inhibitors of mixed lymphocyte
        reaction)
     850706-89-7 CAPLUS
RN
     Benzenesulfonamide, 4,4'-[[2-[(5-fluoro-2-methylphenyl)amino]-5-phenyl-4,6-
CN
     pyrimidinediyl]bis(2-hydrazinyl-1-ylideneethylidyne)]bis[N-methyl- (9CI)
     (CA INDEX NAME)
```

RN 850707-28-7 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(4-fluorophenyl)amino]-5-phenyl-6-[[1-(4-pyridinyl)ethylidene]hydrazino]-4-pyrimidinyl]hydrazono]ethyl]-N-methyl-(9CI) (CA INDEX NAME)

RN 850707-29-8 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(2-fluorophenyl)amino]-5-phenyl-6-[[1-(4-pyridinyl)ethylidene]hydrazino]-4-pyrimidinyl]hydrazono]ethyl]-N-methyl-(9CI) (CA INDEX NAME)

IT 850707-80-1P 850707-81-2P 850708-07-5P

850708-08-6P 850708-09-7P 850708-10-0P 850708-11-1P 850708-12-2P 850708-13-3P

850708-14-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 5-arylpyrimidine derivs. as inhibitors of mixed lymphocyte reaction)

RN 850707-80-1 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(5-fluoro-2-methylphenyl)amino]-6-hydroxy-5-phenyl-(9CI) (CA INDEX NAME)

RN 850707-81-2 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(5-fluoro-2-methylphenyl)amino]-6-hydrazino-5-phenyl-, hydrazone (9CI) (CA INDEX NAME)

$$H_2N-NH$$
  $F$   $N$   $N$   $N$   $N$   $N$   $M$   $M$ 

RN 850708-07-5 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(4-fluorophenyl)amino]-6-hydroxy-5-phenyl- (9CI) (CA INDEX NAME)

RN 850708-08-6 CAPLUS

CN 2-Pyrimidinamine, 4,6-dichloro-N-(4-fluorophenyl)-5-phenyl- (9CI) (CA INDEX NAME)

RN 850708-09-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-chloro-2-[(4-fluorophenyl)amino]-5-phenyl-, hydrazone (9CI) (CA INDEX NAME)

RN 850708-10-0 CAPLUS

CN Benzenesulfonamide, 4-[1-[[6-chloro-2-[(4-fluorophenyl)amino]-5-phenyl-4-pyrimidinyl]hydrazono]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 850708-11-1 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(2-fluorophenyl)amino]-6-hydroxy-5-phenyl- (9CI) (CA INDEX NAME)

RN 850708-12-2 CAPLUS

CN 2-Pyrimidinamine, 4,6-dichloro-N-(2-fluorophenyl)-5-phenyl- (9CI) (CA INDEX NAME)

RN 850708-13-3 CAPLUS

CN 4(1H)-Pyrimidinone, 6-chloro-2-[(2-fluorophenyl)amino]-5-phenyl-, hydrazone (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & C1 & F \\ \hline & N & F \\ H_2N-N & N & NH \end{array}$$

RN 850708-14-4 CAPLUS

CN Benzenesulfonamide, 4-[1-[[6-chloro-2-[(2-fluorophenyl)amino]-5-phenyl-4-pyrimidinyl]hydrazono]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 10 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
AN
     2005:371230 CAPLUS
DN
     142:430289
TΙ
     Preparation of pyrimidine compounds as mixed lymphocyte reaction (MLR)
     inhibitors
IN
     Tsuruoka, Hiroyuki; Matsuda, Akihisa; Sugano, Yuichi; Tatsuta, Toru
.PA
     Sankyo Company, Limited, Japan
SO
     PCT Int. Appl., 350 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     Japanese
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
PΙ
     WO 2005037801
                          A1
                                20050428
                                            WO 2004-JP15955
                                                                    20041021
             AE, AG, AL, AM, AT, AU, AZ,
                                         BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, PT, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     JP 2005145956
                          A2
                                20050609
                                            JP 2004-302344
                                                                    20041018
PRAI JP 2003-360967
                          Α
                                20031021
     MARPAT 142:430289
os
AΒ
     Disclosed is a pyrimidine derivative with excellent MLR inhibitory effect or a
     pharmacol. acceptable salt thereof. Pyrimidine derivs. represented by the
     general formula (I) or pharmacol. acceptable salts thereof [R1 = lower
     alkyl; R2 = each (un)substituted aryl or heterocyclyl; A = NH, O; R3 = H,
     lower alkyl, heterocyclyl, aryl, heterocyclyl, -NHR6 (wherein R6 = lower
     alkyl, cycloalkyl-lower alkyl, aralkyl, each (un)substituted cycloalkyl,
     aryl, or heterocyclyl); R4 = H, lower alkyl, lower alkoxy,
     cycloalkyl-lower alkyl, aralkyl, each (un)substituted aryl or
     heterocyclyl; provided that R3 = R4 \neq H; R5 = H, halo, lower alkyl,
     cycloalkyl, (un) substituted heterocyclyl, NR7R8, OR7 (wherein R7, R8 = H,
     cycloalkyl, (un)substituted aryl or lower alkyl)] are prepared These
     compds. exhibit excellent MLR inhibitory effect and are useful as
     inhibitors of allograft rejection in bone marrow and organ transplant or
     for the prevention and/or treatment of inflammatory diseases,
     organ-specific or organ-nonspecific autoimmune diseases, allergic
     diseases, chronic rheumatism, multiple sclerosis, inflammatory bowel
     disease, diabetes, glomerulonephritis, primary biliary liver cirrhosis,
     chronic active hepatitis, pernicious anemia, chronic thyroiditis, atrophic
     gastritis, myasthenia gravis, psoriasis, Sjoegren's syndrome, systemic
     lupus erythematosus, rhinitis, asthma, or atopic dermatitis. Thus, 0.1
     mmol 4-hydrazino-2,6-bis(2-methoxyphenylamino)pyrimidine was dissolved in
     1 mL ethanol, treated with 0.1 mmol 4-acetylpyridine, and stirred for 18 h
     to give 4-[N'-[1-(pyridin-4-yl)ethylidene]hydrazino]-2,6-bis(2-
     methoxyphenylamino)pyrimidine. N-methyl-4-[1-[[5-phenyl-2-phenylamino-6-
     [4-(pyridin-4-yl)pyrazol-1-yl]pyrimidin-4-yl]hydrazono]ethyl]benzenesulfon
     amide (II) inhibited MLR in human peripheral hemolymphocyte offered from
     two healthy people with IC50 of 1.0 ng/mL.
     850756-40-0P 850756-61-5P 850756-70-6P
```

850757-41-4P 850757-42-5P 850757-43-6P

850757-58-3P 850757-62-9P 850758-21-3P

850758-22-4P 850758-23-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidine compds. as mixed lymphocyte reaction (MLR) inhibitors)

RN 850756-40-0 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(5-fluoro-2-methylphenyl)amino]-5-phenyl-6-[4-(4-pyridinyl)-1H-pyrazol-1-yl]-4-pyrimidinyl]hydrazono]ethyl]-N-methyl-(9CI) (CA INDEX NAME)

RN 850756-61-5 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(2-fluorophenyl)amino]-5-phenyl-4-pyrimidinyl]hydrazono]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 850756-70-6 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(5-fluoro-2-methylphenyl)amino]-5-phenyl-6-(1H-pyrazol-1-yl)-4-pyrimidinyl]hydrazono]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 850757-41-4 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(5-fluoro-2-methylphenyl)amino]-5-phenyl-6-(1H-pyrazol-1-yl)-4-pyrimidinyl]hydrazono]ethyl]-N-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

RN 850757-42-5 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(5-fluoro-2-methylphenyl)amino]-6-(1H-imidazol-1-yl)-5-phenyl-4-pyrimidinyl]hydrazono]ethyl]-N-(2-hydroxyethyl)-(9CI) (CA INDEX NAME)

RN 850757-43-6 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(5-fluoro-2-methylphenyl)amino]-6-(1H-imidazol-1-yl)-5-phenyl-4-pyrimidinyl]hydrazono]ethyl]-N-methyl- (9CI)

(CA INDEX NAME)

RN 850757-58-3 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(5-fluoro-2-methylphenyl)amino]-6-[[2-(2-hydroxyethoxy)ethyl]amino]-5-phenyl-4-pyrimidinyl]hydrazono]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 850757-62-9 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(5-fluoro-2-methylphenyl)amino]-6-[[2-(2-hydroxyethoxy)ethyl]amino]-5-phenyl-, [1-(4-pyridinyl)ethylidene]hydrazone (9CI) (CA INDEX NAME)

RN 850758-21-3 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(4-fluorophenyl)amino]-5-phenyl-6-[[2-(4-pyridinyl)ethyl]amino]-, [1-[4-(methylsulfonyl)phenyl]ethylidene]hydrazone (9CI) (CA INDEX NAME)

RN 850758-22-4 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(4-fluorophenyl)amino]-5-phenyl-6-[[2-(4-pyridinyl)ethyl]amino]-4-pyrimidinyl]hydrazono]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 850758-23-5 CAPLUS

CN Benzenesulfonamide, 4-[1-[[2-[(2-fluorophenyl)amino]-5-phenyl-6-[[2-(4-pyridinyl)ethyl]amino]-4-pyrimidinyl]hydrazono]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

IT 850707-80-1P 850707-81-2P 850708-07-5P 850708-08-6P 850708-11-1P 850708-12-2P 850758-97-3P 850758-98-4P 850759-29-4P 850759-30-7P 850759-38-5P 850760-01-9P 850760-10-0P 850760-48-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrimidine compds. as mixed lymphocyte reaction (MLR) inhibitors)

RN 850707-80-1 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(5-fluoro-2-methylphenyl)amino]-6-hydroxy-5-phenyl-(9CI) (CA INDEX NAME)

RN 850707-81-2 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(5-fluoro-2-methylphenyl)amino]-6-hydrazino-5-phenyl-, hydrazone (9CI) (CA INDEX NAME)

$$H_2N-NH$$
  $F$   $H_2N-N$   $H$   $NH$   $H$ 

RN 850708-07-5 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(4-fluorophenyl)amino]-6-hydroxy-5-phenyl- (9CI) (CA INDEX NAME)

RN 850708-08-6 CAPLUS

CN 2-Pyrimidinamine, 4,6-dichloro-N-(4-fluorophenyl)-5-phenyl- (9CI) (CA INDEX NAME)

RN 850708-11-1 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(2-fluorophenyl)amino]-6-hydroxy-5-phenyl- (9CI) (CA INDEX NAME)

RN 850708-12-2 CAPLUS

CN 2-Pyrimidinamine, 4,6-dichloro-N-(2-fluorophenyl)-5-phenyl- (9CI) (CA INDEX NAME)

RN 850758-97-3 CAPLUS

CN 2-Pyrimidinamine, 4,6-dichloro-N-(5-fluoro-2-methylphenyl)-5-phenyl- (9CI) (CA INDEX NAME)

RN 850758-98-4 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(5-fluoro-2-methylphenyl)amino]-5-phenyl-6-[4-(4-pyridinyl)-1H-pyrazol-1-yl]-, hydrazone (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H_2N-N & F \\ \hline Ph & N \\ N & N \\ \hline N & N \\ \end{array}$$

RN 850759-29-4 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(2-fluorophenyl)amino]-5-phenyl- (9CI) (CA INDEX NAME)

RN 850759-30-7 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(2-fluorophenyl)amino]-5-phenyl-, hydrazone (9CI) (CA INDEX NAME)

RN 850759-38-5 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(5-fluoro-2-methylphenyl)amino]-5-phenyl-6-(1H-pyrazol-1-yl)-, hydrazone (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H_2N-N & F \\ \hline Ph & N \\ N & N \\ \hline N & N \\ \end{array}$$

RN 850760-01-9 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(5-fluoro-2-methylphenyl)amino]-6-(1H-imidazol-1-yl)-5-phenyl-, hydrazone (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ H_2N-N & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\$$

RN 850760-10-0 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(5-fluoro-2-methylphenyl)amino]-6-[[2-(2-hydroxyethoxy)ethyl]amino]-5-phenyl-, hydrazone (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{H}_2\text{N}-\text{NH} \\ \text{Ph} \\ \text{N} \\ \text{HO-CH}_2-\text{CH}_2-\text{O-CH}_2-\text{CH}_2-\text{NH} \\ \end{array}$$

RN 850760-48-4 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(4-fluorophenyl)amino]-5-phenyl-6-[[2-(4-pyridinyl)ethyl]amino]-, hydrazone (9CI) (CA INDEX NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- ANSWER 11 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN L4
- 2005:140796 CAPLUS AN
- DN 142:240444
- TΙ Preparation of 3-(4-pyrimidinylamino)-1H-pyrazoles as protein kinase inhibitors, especially of Aurora-2 and GSK-3
- IN Bebbington, David; Charrier, Jean-damien; Golec, Julian; Miller, Andrew; Knegtel, Ronald
- PA
- SO U.S. Pat. Appl. Publ., 164 pp. CODEN: USXXCO
- DT Patent
- English

FAN. CNT I	A)EP	1
PATENT NO.	KIND 🛭 DATE	APPLICATION
	# <b></b>	<i>j</i>
PI US 2005038023	A1 20050217	<b>∮</b> US 2003-632
PRAI US 2003-632428	<b>1</b> 20030801∕	1

NO. DATE 2428 20030801

PRAI US 2003-632428

MARPAT 142:240444

AΒ The title compds. I [Z1 = N, CR8], Z2 = N, CH; and at least one of Z1 and Z2 = N; Rb, Rc = TR3, LZR3; C2RbRc = (un)substituted fused (hetero)cycle; Q = NR4, O, S, etc.; R1 = TD; D = (un)substituted mono- or bicyclic (hetero)aryl, heterocyclyl, carbocyclyl; T = a bond, alkylidene (un)interrupted by O, S, NR4, CO, etc.; Z = alkylidene; L = O, S, SO, SO2, etc.; R2, R2a = R, TWR6, or C2R2R2a = (un)substituted fused (hetero)cycle; R3 = R, halo, OR, etc.; R = H, (un) substituted aliphatic, (hetero) aryl, heterocyclyl; R4 = R7, COR7, SO2R7, etc.; W = CO, CO2, CONR6, etc.; R6, R7 = H, alkyl; or N(R6)2 or N(R7)2 = heterocyclyl, heteroaryl] were prepared For example, the (pyrazolylamino)quinazoline II was refluxed with thiophenol in tert-BuOH to give III. In bioassays, I inhibited the following kinases with Ki values reported < 20  $\mu$ M: GSK-3 $\beta$ , AURORA-2, CDK-2, ERK2, AKT, and human Src kinase. I are useful for the treatment of diseases associated with protein kinases, such as diabetes, cancer, and Alzheimer's disease (no data).

IT 438205-79-9P 438205-80-2P 438205-86-8P 438205-87-9P

> RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(protein kinase inhibitor; preparation of (pyrimidinylamino)pyrazoles as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

- RN 438205-79-9 CAPLUS
- CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-(5-methyl-1H-pyrazol-3-yl)-6-(3-nitrophenyl) - (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 438205-80-2 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-(5-methyl-1H-pyrazol-3-yl)-6-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 438205-86-8 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-[5-(1,1-dimethylethyl)-1H-pyrazol-3-yl]-6-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 438205-87-9 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-6-(3-nitrophenyl)-N4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

```
ANSWER 12 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
AN
     2005:120897 CAPLUS
DN
     142:219296
ΤI
     Preparation of 2-aminophenyl-4-phenylpyrimidines as kinase inhibitors
IN
     Wang, Shudong; McLachlan, Janice; Gibson, Darren; Causton, Ashley; Turner,
     Nicholas; Fischer, Peter
PA
     Cyclacel Limited, UK
SO
     PCT Int. Appl., 115 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                  DATE
                                               APPLICATION NO.
                                                                       DATE
PΙ
     WO 2005012262
                           A1
                                  20050210
                                              WO 2004-GB3284
                                                                       20040730
             AE, AG, AL, AM, AT, AU, AZ,
                                           ∕BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK,
                                           DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
     AU 2004261484
                                  20050210
                           A1
                                              AU 2004-261484
                                                                       20040730
     CA 2533474
                           AΑ
                                  20050210
                                               CA 2004-2533474
                                                                       20040730
     EP 1648875
                           A1
                                  20060426
                                               EP 2004-743610
                                                                       20040730
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
     BR 2004012347
                           Α
                                  20060905
                                              BR 2004-12347
                                                                       20040730
     CN 1860104
                           Α
                                  20061108
                                               CN 2004-80028477
                                                                       20040730
PRAI GB 2003-17841
                           Α
                                  20030730
     GB 2003-18345
                           Α
                                  20030805
     WO 2004-GB3284
                           W
                                  20040730
os
     MARPAT 142:219296
AB
     Title compds. I [Z = (un)] substituted alkyl, N; R1-2 = (CH2)0-4R11, H, R11,
     etc.; R3, R5 = H; R4 = H, R11; R6 = H, alkyl; R7, R9 = H, R11; R11 = halo,
     NO2, CN, etc.] are prepared For instance, [4-(3-Aminophenyl)pyrimidin-2-
     yl][4-(2-methoxyethoxy)phenyl]amine (II) is prepared from
     3-aminoacetophenone, N,N-dimethylformamide di-Me acetal, 2-methoxyethanol
     and 4-aminophenol. II exhibits IC50 = 0.018 μM against Cdk9/Cyclin T1.
     I are tyrosine kinase inhibitors and useful for the treatment of, e.g.,
     rheumatoid arthritis and leukemia.
     839727-08-1P, 3-[2-(3-Fluorophenylamino)pyrimidin-4-yl]phenol
     839727-21-8P, [3-[2-[(3-Fluorophenyl)amino]pyrimidin-4-
     yl]phenyl]methanol 839727-22-9P, (3-Fluorophenyl)[4-(3-
     methoxyphenyl)pyrimidin-2-yl]amine 839727-23-0P,
     (3-Fluorophenyl) [4-(4-methoxyphenyl)pyrimidin-2-yl]amine
     839727-29-6P, (4-Fluorophenyl)[4-(3-nitrophenyl)pyrimidin-2-
     yl]amine 839727-30-9P, [4-(3-Aminophenyl)pyrimidin-2-yl](4-
     fluorophenyl)amine 839727-37-6P, (4-Chlorophenyl)[4-(3-
     chlorophenyl)pyrimidin-2-yl]amine 839727-66-1P,
     [4-(2,5-Dimethylphenyl)pyrimidin-2-yl](3-fluorophenyl)amine
     839727-67-2P, (3-Fluorophenyl)[4-(3-nitrophenyl)pyrimidin-2-
     yl]amine 839727-73-0P, 3-[2-[[3,5-Bis(trifluoromethyl)phenyl]ami
     no]pyrimidin-4-yl]phenol
```

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-aminophenyl-4-phenylpyrimidines as kinase inhibitors) RN 839727-08-1 CAPLUS

CN Phenol, 3-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 839727-21-8 CAPLUS

CN Benzenemethanol, 3-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 839727-22-9 CAPLUS

CN 2-Pyrimidinamine, N-(3-fluorophenyl)-4-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 839727-23-0 CAPLUS

CN 2-Pyrimidinamine, N-(3-fluorophenyl)-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 839727-29-6 CAPLUS

CN 2-Pyrimidinamine, N-(4-fluorophenyl)-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 839727-30-9 CAPLUS

CN 2-Pyrimidinamine, 4-(3-aminophenyl)-N-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 839727-37-6 CAPLUS

CN 2-Pyrimidinamine, 4-(3-chlorophenyl)-N-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

RN 839727-66-1 CAPLUS

CN 2-Pyrimidinamine, 4-(2,5-dimethylphenyl)-N-(3-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 839727-67-2 CAPLUS

CN 2-Pyrimidinamine, N-(3-fluorophenyl)-4-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 839727-73-0 CAPLUS

CN Phenol, 3-[2-[[3,5-bis(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 13 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
AN
     2005:14169 CAPLUS
     142:114470
DN
     Preparation of sulfonylated peptide derivatives for treating rheumatoid
ΤI
     arthritis
     Yednock, Theodore A.; Freedman, Stephen B.; Lieberburg, Ivan; Pleiss,
IN
     Michael A.; Konradi, Andrei W.; Shopp, George; Messersmith, Elizabeth
     Elan Pharmaceuticals, Inc., USA
PA
SO
     PCT Int. Appl., 736 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 2
     PATENT NO.
                          KIND
                                  ĎATE
                                               APPLICATION NO.
                                                                        DATE
PΙ
     WO 2005000246
                           A2
                                  20050106
                                               WO 2004-US20280
                                                                        20040625
     WO 2005000246
                           A3
                                  2005112A
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
         TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
              SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
     AU 2004251754
                           A2
                                  20050106
                                               AU 2004-251754
                                                                        20040625
     AU 2004251754
                           A1
                                  20050106
     CA 2529873
                                  20050106
                           AΑ
                                               CA 2004-2529873
                                                                        20040625
     US 2005065192
                                  20050324
                                               US 2004-875282
                           A1
                                                                        20040625
     US 2005074451
                           A1
                                  20050407
                                               US 2004-875469
                                                                        20040625
     EP 1635822
                           A2
                                  20060322
                                               EP 2004-777033
                                                                        20040625
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRAI US 2003-482211P
                           Ρ
                                  20030625
     WO 2004-US20280
                           W
                                  20040625
os
     MARPAT 142:114470
AΒ
     The invention relates to methods and compns. for treating rheumatoid
     arthritis by administering a combination therapy comprising methotrexate
     and an antibody to \alpha 4 integrin or an immunol. active antigen binding
     fragment in therapeutically effective amts. Compds. R1SO2NR2CHR3-Q-
     CHR5CO2H [R1 is (un)substituted alkyl, aryl, cycloalkyl, heterocyclyl or
     heteroaryl; R2 is H, (un) substituted cycloalkenyl or any group given for
     R1; R3 is H or any group given for R1; R2 can combine with R1 or R3 to
     form an (un) substituted heterocyclic group; R5 is -(CH2)1-4-Ar-R5', where
     R5' is -O-Z-NR8R8' or -O-Z-R8'', Ar is (un)substituted aryl or heteroaryl,
     Z is CO or SO2, R8, R8' are H, (un) substituted alkyl, cycloalkyl or
     heterocyclyl or NR8R8' is (un) substituted heterocyclyl, and R8'' is
     (un) substituted heterocyclyl; Q is -C(X)NR7-, where R7 is H or alkyl and X
     is O or S] are claimed for use in combination therapy.
                                                                 Thus,
     N-tosyl-L-prolyl-4-(dimethylcarbamoyloxy)-L-phenylalanine Et ester was
     prepared by acylation of Ts-Pro-Tyr-OEt with dimethylcarbamoyl chloride.
     Compds. of the invention have binding affinity to \alpha 4\beta 1 (IC50
     \leq 15 \muM).
IT
     285139-65-3P 285140-62-7P
```

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of sulfonylated peptide derivs. for treating rheumatoid arthritis)

RN 285139-65-3 CAPLUS

CN L-Tyrosine, N-[2-[(4-chlorophenyl)methylamino]-5-(2-methylphenyl)-4-pyrimidinyl]-, dimethylcarbamate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 285140-62-7 CAPLUS

CN [1,1'-Biphenyl]-4-propanoic acid,  $\alpha$ -[[2-[(4-chlorophenyl)methylamino]-5-(2,4,6-trimethylphenyl)-4-pyrimidinyl]amino]-2',6'-dimethoxy-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

```
ANSWER 14 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
ΑN
      2005:14167 CAPLUS
DN
      142:114469
ΤI
      Preparation of sulfonylated peptide derivatives for treating rheumatoid
      arthritis
IN
      Yednock, Theodore A.; Freedman, Stephen B.; Lieberburg, Ivan; Pleiss,
      Michael A.; Konradi, Andrei W.; Shopp, George; Messersmith, Elizabeth
PΑ
      Elan Pharmaceuticals, Inc., USA
SO
      PCT Int. Appl., 647 pp.
      CODEN: PIXXD2
DT
      Patent
LA
      English
FAN.CNT 2
      PATENT NO.
                              KIND/
                                       DATE
                                                     APPLICATION NO.
                                                                                  DATE
                                                     -----
                                                                                  _____
                               A2
PΙ
      WO 2005000244
                                       20050106
                                                     WO 2004-US20240
                                                                                  20040625
      WO 2005000244
                               АЗ
                                       20050929
               AE, AG, AL, AM, AT, AU, AZ,
                                                 BA, BB, BG, BR, BW, BY, BZ, CA, CH,
          W: AE, AG, AL, AM, AT, AU, AZ; BA, BB, BG, BK, BW, BI, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, FD, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, FF FS, FT, FR, GR, GR, HU, TE, TT, LU, MC, NI, PL, PT, RO, SE,
               EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
                SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
               SN, TD, TG
      AU 2004251750
                               A2
                                       20050106
                                                     AU 2004-251750
                                                                                  20040625
      AU 2004251750
                               A1
                                       20050106
      CA 2528723
                               AA
                                       20050106
                                                     CA 2004-2528723
                                                                                  20040625
      US 2005065192
                               A1
                                       20050324
                                                     US 2004-875282
                                                                                  20040625
      US 2005074451
                                       20050407
                               A1
                                                     US 2004-875469
                                                                                  20040625
      EP 1635871
                                       20060322
                               A2
                                                     EP 2004-777008
                                                                                  20040625
              AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
               IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRAI US 2003-482211P
                                       20030625
                               Р
      WO 2004-US20240
                               W
                                       20040625
AB
      The invention relates to methods and compns. for treating rheumatoid
      arthritis by administering a combination therapy comprising methotrexate
      and an antibody to \alpha 4 integrin or an immunol. active antigen binding
      fragment in therapeutically effective amts. Compds. include those
      described by formula R1SO2NR2CHR3-Q-CHR5CO2H [R1 is (un)substituted alkyl,
      aryl, cycloalkyl, heterocyclyl or heteroaryl; R2 is H, (un) substituted
      cycloalkenyl or any group given for R1; R3 is H or any group given for R1;
      R2 can combine with R1 or R3 to form an (un) substituted heterocyclic
      group; R5 is -(CH2)1-4-Ar-R5', where R5' is -O-Z-NR8R8' or -O-Z-R8'', Ar
      is (un)substituted aryl or heteroaryl, Z is CO or SO2, R8, R8' are H,
      (un) substituted alkyl, cycloalkyl or heterocyclyl or NR8R8' is
      (un) substituted heterocyclyl, and R8'' is (un) substituted heterocyclyl; O
      is -C(X)NR7-, where R7 is H or alkyl and X is O or S]. Thus,
      N-tosyl-L-prolyl-4-(dimethylcarbamoyloxy)-L-phenylalanine Et ester was
      prepared by acylation of Ts-Pro-Tyr-OEt with dimethylcarbamoyl chloride.
      Compds. of the invention have binding affinity to \alpha 4\beta 1 (IC50
      \leq 15 \muM).
      285139-65-3P
IT
      RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
      (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
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(Uses)

(preparation of sulfonylated peptide derivs. for treating rheumatoid arthritis)

RN

285139-65-3 CAPLUS L-Tyrosine, N-[2-[(4-chlorophenyl)methylamino]-5-(2-methylphenyl)-4-CN pyrimidinyl]-, dimethylcarbamate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 15 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:857162 CAPLUS

DN 141:350185

TI Preparation of pyrimidine derivatives with lysophosphatidic acid acyltransferase  $\beta$  (LPAAT- $\beta$ ) inhibitory activity

IN Bhatt, Rama; Gong, Baoqing; Hong, Feng; Jenkins, Scott A.; Klein, J. Peter; Kohm, Cory T.; Tulinsky, John

PA Cell Therapeutics, Inc., USA

SO U.S. Pat. Appl. Publ., 80 pp., which CODEN: USXXCO

DT Patent

LA English

FAN. CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2004204386	A1	20041014	US 2003-671070	20030924
PRAI US 2002-419694P	P	20021017		
US 2003-460776P	P	20030404		

OS MARPAT 141:350185

AB The title compds. I [X, Y, Z = N, CH, or CR with the proviso that two of X, Y and Z are N; R = alkyl, alkoxy, Cl, Br, (substituted)amino; Q = NR', R'N-(CH2)n, (CH2)n-NR', O, O-(CH2)n, (CH2)n-O, S, S-(CH2)n, or (CH2)n-S; n = 1-10; R' = H or alkyl; R1 = H, OH, alkyl, alkoxy, Cl, F, Br, etc.; R2, R7 = H, OH, alkyl, alkoxy, Cl, F, Br, I, etc.; R3 = H, alkyl, alkoxy, Cl, CCl3, (substituted)amino; R4, R5, R6 = H, OH, alkyl, alkenyl, alkynyl, alkoxy, etc. or R4, R5 or R5, R6 are taken together with benzene ring to form a heterocycle] are prepared as lysophosphatidic acid acyltransferase  $\beta$  (LPAAT- $\beta$ ) inhibitors for the treatment of diseases related to cell proliferation, such as cancer. For example, reaction of 6-chloro-N4-(4-methylphenyl)-pyrimidine-2,4-diamine (preparation given) with 5-chloro-2-methoxy-Ph boronic acid yielded compound II. The latter exhibits an IC50 = 0.12  $\mu$ M in the LPAAT- $\beta$  assay.

IT 710334-91-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidine derivs. with lysophosphatidic acid acyltransferase  $\beta$  (LPAAT- $\beta$ ) inhibitory activity)

RN 710334-91-1 CAPLUS

CN 2,4-Pyrimidinediamine, 6-(5-chloro-2-methoxyphenyl)-N2-(4-chlorophenyl)-(9CI) (CA INDEX NAME)

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ANSWER 16 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
AN
     2004:430750 CAPLUS
DN
     141:7129
ΤI
     Preparation of 4-heteroarylpyrimidines as specific cyclin-dependent kinase
     inhibitors for treating viruses
IN
     Wang, Shudong; Meades, Christopher; Wood, Gavin; Blake, David; Fischer,
     Peter
PΑ
     Cyclacel Limited, UK
SO
     PCT Int. Appl., 142 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                              APPLICATION NO.
                                                                       DATE
PΙ
     WO 2004043467
                           A1
                                20040527
                                              WO 2003-GB4977
                                                                       20031114
             AE, AG, AL, AM,
                              AT, AU, AZ,
                                           BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, LM, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2003283585
                           Α1
                                  20040603
                                              AU 2003-283585
                                                                       20031114
     EP 1581231
                           A1
                                  20051005
                                              EP 2003-775562
                                                                       20031114
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     US 2005288307
                           A1
                                  20051229
                                              US 2005-129198
                                                                       20050513
PRAI GB 2002-26582
                           Α
                                  20021114
     WO 2003-GB4977
                           W
                                  20031114
os
     MARPAT 141:7129
AB
     Title compds. I [wherein one of X1 and X2 = S, and the other of X1 and X2
     = N so as to form a thiazolyl ring, R2 = independently as defined below
     for R1 and R3; one of X1 and X2 = S, and the other of X1 and X2 = NH and
     derivs. so as to form a 4,5-dihydrothiazolyl ring; R2 = oxo; the bond
     between C and R2 = double; Z = NH, NHCO, NHSO2, NHCH2, CH2, CH2CH2, CH:CH;
     R1, R3 = independently H, halo, NO2, CN, OH and derivs., NH2 and derivs.,
     CO2H and derivs., CONH2 and derivs., SO3H, (un) substituted ar/alkyl, aryl,
     heterocyclyl, etc.; R4, R5, R6, R7, R8 = independently H, halo, NO2, CN,
     OH and derivs., NH2 and derivs., alkylheteroaryl, SO3H, SO2NH2, CF3,
     (un) substituted lower alkyl; and their pharmaceutically acceptable salts]
     were prepared for use in the treatment of viral disorders. For example, II
     was prepared by cyclocondensation of 3-Dimethylamino-1-(2,4-dimethylthiazol-
     5-yl)propenone (preparation given) with N-(3-Nitrophenyl)guanidine nitrate
     (preparation given) in 2-methoxyethanol in the presence of NaOH. Selected I
     showed high degree of selectivity for inhibition of CDKs. II displayed an
     average IC50 of 0.23 µM against CDK2-Cyclin El kinase. Thus, I are useful
     for treating cytomegalovirus, herpes simplex, HIV-I, and varicella-zoster
     virus.
ΤT
     364334-28-1P, [4-(2,4-Dimethylthiazol-5-yl)-6-phenylpyrimidin-2-
     yl](4-fluorophenyl)amine 364334-31-6P, [4-(2,4-Dimethylthiazol-5-
     yl)-6-(4-trifluoromethylphenyl)pyrimidin-2-yl](4-fluorophenyl)amine
     364334-32-7P, (4-Chlorophenyl)[4-(2,4-dimethylthiazol-5-yl)-6-(4-
     trifluoromethylphenyl)pyrimidin-2-yl]amine 364334-35-0P,
     [4-(2,4-Dimethylthiazol-5-yl)-6-(3-trifluoromethylphenyl)pyrimidin-2-yl](4-
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fluorophenyl)amine 364334-36-1P, 4-[6-(2,4-Dimethylthiazol-5-yl)-2-(4-fluorophenylamino)pyrimidin-4-yl]-2,6-dimethoxyphenol
364334-37-2P, 4-[6-(2,4-Dimethylthiazol-5-yl)-2-(4fluorophenylamino)pyrimidin-4-yl]phenol
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
 (anti-viral agent; preparation of 4-heteroarylpyrimidines as specific cyclin-dependent kinase inhibitors for treating viruses)
364334-28-1 CAPLUS

RN 364334-28-1 CAPLUS
CN 2-Pyrimidinamine, 4-(2,4-dimethyl-5-thiazolyl)-N-(4-fluorophenyl)-6-phenyl(9CI) (CA INDEX NAME)

RN 364334-31-6 CAPLUS

CN 2-Pyrimidinamine, 4-(2,4-dimethyl-5-thiazolyl)-N-(4-fluorophenyl)-6-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 364334-32-7 CAPLUS

CN 2-Pyrimidinamine, N-(4-chlorophenyl)-4-(2,4-dimethyl-5-thiazolyl)-6-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 364334-35-0 CAPLUS

CN 2-Pyrimidinamine, 4-(2,4-dimethyl-5-thiazolyl)-N-(4-fluorophenyl)-6-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 364334-36-1 CAPLUS

CN Phenol, 4-[6-(2,4-dimethyl-5-thiazolyl)-2-[(4-fluorophenyl)amino]-4-pyrimidinyl]-2,6-dimethoxy- (9CI) (CA INDEX NAME)

RN 364334-37-2 CAPLUS

CN Phenol, 4-[6-(2,4-dimethyl-5-thiazolyl)-2-[(4-fluorophenyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 17 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
ΑN
      2004:412938 CAPLUS
DN
      140:423692
 ΤI
      Pyridine and pyrimidine derivatives and their compositions, useful as
      inhibitors of JAK and other protein kinases
 IN
      Bethiel, Randy S.; Moon, Young Choon
PA
      Vertex Pharmaceuticals Incorporated, USA
· SO
      PCT Int. Appl., 104 pp.
      CODEN: PIXXD2
DT
      Patent
LΑ
      English
 FAN.CNT 1
      PATENT NO.
                             KIND
                                     DATE
                                                  APPLICATION NO.
                                                                            DATE
      WO 2004041810
PΤ
                              A1
                                    20040521
                                                  WO 2003-US35188
                                                                            20031105
           W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
               CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,
               NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
          RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
               TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
      CA 2507406
                                                  CA 2003-2507406
                                     20040521
                              AA
                                                                            20031105
      AU 2003286895
                                     20040607
                              A1
                                                  AU 2003-286895
                                                                            20031105
      US 2004176271
                              A1
                                     20040909
                                                  US 2003-702113
                                                                            20031105
                                     20050810
      EP 1560824
                              A1
                                                  EP 2003-778111
                                                                            20031105
               AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
               IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
      JP 2006508107
                              T2
                                     20060309
                                                  JP 2004-550489
                                                                            20031105
 PRAI US 2002-424043P
                              Ρ
                                     20021105
      WO 2003-US35188
                              W
                                     20031105
OS
      MARPAT 140:423692
AΒ
      The invention provides compds. of formula I or pharmaceutically acceptable
      salts thereof. The invention also provides pharmaceutically acceptable
      compns. comprising I, and methods of utilizing I and their compns. in the
      treatment of various protein kinase-mediated disorders. In compds. I, R1
      is Q-Arl; Q is a bond or C1-2 alkylidene chain wherein one methylene unit
      is optionally replaced by O, NR, NRCO, NRCONR, NRCO2, CO, CO2, CONR,
      OC(O)NR, SO2, SO2NR, NRSO2, NRSO2NR, C(O)C(O), or C(O)CH2C(O); R is H or
      (un) substituted aliphatic; Arl is (un) substituted, (poly) (un) saturated, 5- to
      7-membered monocyclic ring having 0-3 N/O/S heteroatoms, or 8- to
      12-membered bicyclic ring system having 0-5 N/O/S heteroatoms; Z1 is N or
      CH; Z7 is N or CURy; T, U are bond or (un)saturated C1-6 alkylidene chain,
      wherein up to two methylene units of the chain are optionally and
      independently replaced by CO, CO2, COCO, CONR, OCONR, NRNR, NRNRCO, NRCO,
      NRCO2, NRCONR, SO, SO2, NRSO2, SO2NR, NRSO2NR, O, S, or NR; Rx, Ry are
      independently halogen, CN, NO2, or R'; Z2, Z5, and Z6 are independently N
      or CH, provided that no more that 2 of them are N; Z3 is CR3; Z4 is CR4;
      wherein one of R3 and R4 is Ru and the other is OR'; Ru is (CH2)tCN,
      (CH2)tNO2, (CH2)tNR2, (CH2)tNRCOR, (CH2)tCONR2, (CH2)tCO2R, (CH2)tAr2,
      etc.; t is 0-2; Ar2 is an (un)substituted, (poly)(un)saturated 5- to
      7-membered, monocyclic ring having 0-3 N/O/S heteroatoms; and R' is H,
      (un) substituted aliphatic or (bi) (hetero) cyclic. Approx. 190 compds. I are
      claimed individually. A general multi-step preparation is described in
      examples, including step combinations and final product mol. wts. for
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approx. 30 invention compds., including II. In a JAK3 inhibition assay, several invention compds. had Ki values less than 0.1  $\mu M$ . Similar potencies were obtained for some compds. against CDK2, JNK3, SYK, and GSK-3. 691894-96-9P 691894-97-0P 691895-06-4P ΙT 691895-07-5P 691895-08-6P 691895-10-0P 691895-24-6P 691895-25-7P 691895-28-0P 691895-29-1P 691895-30-4P 691895-32-6P 691895-36-0P 691895-38-2P 691895-54-2P 691895-55-3P 691895-65-5P 691895-66-6P 691895-67-7P 691895-68-8P 691896-10-3P 691896-11-4P 691896-14-7P 691896-16-9P 691896-19-2P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyridine and pyrimidine derivs. as inhibitors of JAK and other protein kinases)

RN 691894-96-9 CAPLUS

CN

2-Pyrimidinamine, 4-(3-amino-4-methoxyphenyl)-N-(3-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 691894-97-0 CAPLUS

CN 2-Pyrimidinamine, 4-(3-amino-4-methoxyphenyl)-N-(3-chlorophenyl)- (9CI) (CA INDEX NAME)

RN 691895-06-4 CAPLUS

CN 2-Pyrimidinamine, N-(4-fluorophenyl)-4-(4-methoxy-3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 691895-07-5 CAPLUS
CN 2-Pyrimidinamine, N-(4-chlorophenyl)-4-(4-methoxy-3-nitrophenyl)- (9CI)
(CA INDEX NAME)

RN 691895-08-6 CAPLUS
CN 2-Pyrimidinamine, N-(3-fluorophenyl)-4-(4-methoxy-3-nitrophenyl)- (9CI)
(CA INDEX NAME)

RN 691895-10-0 CAPLUS CN 2-Pyrimidinamine, N-(3-chlorophenyl)-4-(4-methoxy-3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 691895-24-6 CAPLUS
CN Benzamide, 5-[2-[(4-fluorophenyl)amino]-4-pyrimidinyl]-2-hydroxy- (9CI) (CA INDEX NAME)

RN 691895-25-7 CAPLUS
CN Benzamide, 5-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]-2-hydroxy- (9CI) (CA INDEX NAME)

RN 691895-28-0 CAPLUS
CN Benzamide, 5-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-hydroxy- (9CI) (CA INDEX NAME)

RN 691895-29-1 CAPLUS
CN Benzamide, 5-[2-[(4-chlorophenyl)amino]-4-pyrimidinyl]-2-methoxy- (9CI)
(CA INDEX NAME)

RN 691895-30-4 CAPLUS
CN Benzamide, 5-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-methoxy- (9CI)
(CA INDEX NAME)

RN 691895-32-6 CAPLUS
CN Benzamide, 5-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]-2-methoxy- (9CI) (CA INDEX NAME)

RN 691895-36-0 CAPLUS

CN Benzamide, 5-[2-[(3,4-difluorophenyl)amino]-4-pyrimidinyl]-2-methoxy-(9CI) (CA INDEX NAME)

RN 691895-38-2 CAPLUS

CN Benzamide, 5-[2-[(4-fluorophenyl)amino]-4-pyrimidinyl]-2-methoxy- (9CI) (CA INDEX NAME)

RN 691895-54-2 CAPLUS

CN Benzamide, 5-[2-[(4-fluorophenyl)amino]-4-pyrimidinyl]-2-(1-methylethoxy)-(9CI) (CA INDEX NAME)

RN 691895-55-3 CAPLUS

CN Benzamide, 5-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]-2-(1-methylethoxy)-(9CI) (CA INDEX NAME)

RN 691895-65-5 CAPLUS

CN Benzamide, 5-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-(1-methylethoxy)-(9CI) (CA INDEX NAME)

RN 691895-66-6 CAPLUS

CN Benzamide, 5-[2-[(3,4-difluorophenyl)amino]-4-pyrimidinyl]-2-(1-methylethoxy)- (9CI) (CA INDEX NAME)

RN 691895-67-7 CAPLUS

CN Benzamide, 5-[2-[(4-chloro-3-cyanophenyl)amino]-4-pyrimidinyl]-2-(1-methylethoxy)- (9CI) (CA INDEX NAME)

RN 691895-68-8 CAPLUS

CN Benzamide, 5-[2-[(3,5-dichlorophenyl)amino]-4-pyrimidinyl]-2-(1-methylethoxy)- (9CI) (CA INDEX NAME)

RN 691896-10-3 CAPLUS

CN Phenol, 4-[2-[(4-fluorophenyl)amino]-4-pyrimidinyl]-2-nitro- (9CI) (CA INDEX NAME)

RN 691896-11-4 CAPLUS

CN Phenol, 4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]-2-nitro- (9CI) (CA INDEX NAME)

RN 691896-14-7 CAPLUS

CN Phenol, 4-[2-[(3-chloro-4-methoxyphenyl)amino]-4-pyrimidinyl]-2-nitro-(9CI) (CA INDEX NAME)

RN 691896-16-9 CAPLUS

CN Phenol, 4-[2-[(3-fluorophenyl)amino]-4-pyrimidinyl]-2-nitro- (9CI) (CA INDEX NAME)

RN 691896-19-2 CAPLUS

CN Phenol, 2-amino-4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

### 10/501,445

L4 ANSWER 18 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:303311 CAPLUS

DN 141:64387

TI Synthesis, SAR, and antitumor properties of diamino-C,N-diarylpyrimidine positional isomers: inhibitors of lysophosphatidic acid acyltransferase- $\beta$ 

AU Gong, Baoqing; Hong, Feng; Kohm, Cory; Jenkins, Scott; Tulinsky, John; Bhatt, Rama; de Vries, Peter; Singer, Jack W.; Klein, Peter

CS Cell Therapeutics, Inc., Seattle, WA, 98119, USA

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(9), 2303-2308 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

OS CASREACT 141:64387

AB 2,4-Diamino-N4,6-diarylpyrimidines were identified as potent, isoform specific inhibitors of lysophosphatidic acid acyltransferase- $\beta$  (LPAAT- $\beta$ ). Active inhibitors also blocked proliferation of tumor cell lines in vitro. The effect of one of the synthesized compds. (2j) in an in vivo tumor model was investigated.

TT 710334-91-1P 710334-92-2P RL: PAC (Pharmacological activity); PR

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis, SAR, and antitumor properties of diamino-C,N-diarylpyrimidine positional isomers, inhibitors of lysophosphatidic acid acyltransferase- $\beta$ )

RN 710334-91-1 CAPLUS

CN 2,4-Pyrimidinediamine, 6-(5-chloro-2-methoxyphenyl)-N2-(4-chlorophenyl)-(9CI) (CA INDEX NAME)

RN 710334-92-2 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-bromophenyl)-6-(5-chloro-2-methoxyphenyl)-(9CI) (CA INDEX NAME)

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:182368 CAPLUS

DN 140:229401

TI Three hybrid assay system for isolating ligand-binding polypeptides and for isolating small mol. ligands

IN Come, Jon H.; Becker, Frank; Kley, Nikolai A.; Reichel, Christoph

PA Gpc Biotech Inc., USA; Gpc Biotech AG

SO U.S. Pat. Appl. Publ., 238 pp., Cont.-in-part of U.S. Ser. No. 91,177. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 6

11211	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	US 2004043388	A1	20040304	US 2002-234985	20020903
	US 7135550	B2	20061114		
	US 2003165873	<b>A</b> 1	20030904	US 2002-91177	20020304
	US 2004266854	<b>A</b> 1	20041230	US 2004-820453	20040407
PRAI	US 2001-272932P	P	20010302		
	US 2001-278233P	P	20010323	X )	
	US 2001-329437P	P	20011015		
	US 2002-91177	<b>A</b> 2	20020304	/	
	US 2001-336962P	P	20011203	. /	
	WO 2002-US6677	A2	20020304	ŧ	
	US 2002-234985	A2	20020903		
	WO 2002-US33052	A2	20021015		
	US 2003-460921P	Ρ.	20030407		
	US 2003-531872P	P	20031223		

AB The invention provides compns. and methods for isolating ligand-binding polypeptides for a user-specified ligand, and for isolating small mol. ligands for a user-specified target polypeptide using an improved class of hybrid ligand compds. Preparation of compds., e.g a methotrexate moiety linked by a polyethylene gycol moiety to dexamethasone, is described.

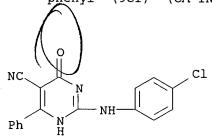
IT 273920-44-8D, conjugates.

RL: BUU (Biological use, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(three hybrid assay system for isolating ligand-binding polypeptides and for isolating small mol. ligands)

RN 273920-44-8 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-[(4-chlorophenyl)amino]-1,4-dihydro-4-oxo-6-phenyl- (9CI) (CA INDEX NAME)



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ANSWER 20 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
    2004:162676 CAPLUS
AN
DN
     140:199343
     Preparation of aminopyrimidine derivatives as protein kinase inhibitors
ΤI
IN
     Cochran, John; Green, Jeremy; Hale, Michael R.; Ledford, Brian; Maltais,
     Francois; Nanthakumar, Suganthini
PA
    Vertex Pharmaceuticals Incorporated, USA
SO
     PCT Int. Appl., 179 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                             APPLICATION NO.
                                                                      DATE
    WO 2004016597
PI
                          A2
                                 20040226
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                                                                      20030812
    WO 2004016597
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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     CA 2495386
                                 20040226
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                                             CA 2003-2495386
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    AU 2003262642
                          A1
                                 20040303
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                          Α1
                                 20040603
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                                                                      20030812
    BR 2003013397
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                                             BR 2003-13397
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     EP 1546117
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                                             EP 2003-788433
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             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     JP 2006506462
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                                 20060223
                                             JP 2005-502048
                                                                      20030812
    NO 2005001207
                          Α
                                 20050518
                                             NO 2005-1207
                                                                      20050308
PRAI US 2002-403256P
                          Ρ
                                 20020814
    US 2002-416802P
                           Ρ
                                 20021008
    WO 2003-US25333
                          W
                                 20030812
OS
    MARPAT 140:199343
    Title compds. I [wherein B = 6-membered aryl ring with 0-3 N atoms, Z1, Z2
     = independently N, CH; T, Q = independently saturated or unsatd. alkylidene; U
     = NH and derivs., NHCO2 and derivs., o, CONH and derivs., CO, CO2, OCO,
     NHSO2 and derivs., SO2NH and derivs., SO2, etc.; m, n = independently 0 or
     1; p = 0-4; R1 = R or Ar; R = H, (un) substituted aliphatic group; Ar =
     (un) substituted 6-10 membered aryl ring, 5-10 membered heteroaryl ring
     having 1-4 heteroatoms, or a 3-10 heterocyclyl membered ring having 1-4
     heteroatoms; R3 = R, Ar, (CH2)yCH(R5)2 or CN; y = 0-6; R2 = (CH2)yCH(R5)2,
     (CH2)yCH(R4)CH(R5)2; R4 = R, (CH2)wOR, (CH2)wN(R)2 \text{ or } (CH2)wSR; w = 0-4;
     R5 = independently Ar, OR, CO2R, SR, SO2R, CN, N(Ar)(R), (un)substituted
     aliphatic, etc.; R6 = independently R, F, C1, NH2 and derivs., OR, SR, SO2R,
     NRSO2R, CN, SO2N(R)2, etc.; and their pharmaceutically acceptable salts]
     were prepared as protein kinase inhibitors (no data). For example, II was
     prepared in 3 steps by Pd-cross coupling of 2,4-dichloro-5-fluoropyrimidine
     with 4-methoxycarbonylphenyl boronic acid (III), acylation of
     (S)-3-chlorophenyl glycinol with III, and alkylation of isopropylamine
     with 2-chloropyrimidine intermediate. I and their formulations are useful
     for treating or lessening the severity of a variety of disorders,
     including stroke, inflammatory disorders, autoimmune diseases such as SLE
```

lupus and psoriasis, proliferative disorders such as cancer, and conditions associated with organ transplantation (no data).

IT 663612-09-7P 663612-13-3P 663612-15-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(protein kinase inhibitor; preparation of 6-membered heterocycles, in particular aminopyrimidines as protein kinase inhibitors)

RN 663612-09-7 CAPLUS

CN 4-Morpholineacetamide, N-[4-[2-[(3-chlorophenyl)amino]-4-pyrimidinyl]phenyl]- $\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 663612-13-3 CAPLUS

CN 4-Morpholineacetamide,  $\alpha$ -phenyl-N-[4-[2-[[3-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)

RN 663612-15-5 CAPLUS

CN 4-Morpholineacetamide, N-[4-[2-[(3-bromophenyl)amino]-4-pyrimidinyl]phenyl]- $\alpha$ -phenyl- (9CI) (CA INDEX NAME)

#### 10/501,445

L4 ANSWER 21 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:1001978 CAPLUS

DN 140:314405

TI A novel series of potent and selective IKK2 inhibitors

AU Bingham, Alistair H.; Davenport, Richard J., Gowers, Lewis; Knight, Roland L.; Lowe, Christopher; Owen, David A.; Parry, David M.; Pitt, Will R.

CS Celltech R&D Ltd, Great Abington, Cambridge, CB16GS, UK

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(2), 409-412 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

OS CASREACT 140:314405

AB A novel series of aminopyrimidine IKK2 inhibitors have been developed which show excellent in vitro inhibition of this enzyme and good selectivity over the IKK1 isoform. The relative potency and selectivity of these compds. has been rationalized using QSAR and structure-based modeling.

IT 677753-07-0P 677753-13-8P 677753-14-9P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and QSAR studies of series of potent and selective aminopyrimidine IKK2 inhibitors)

RN 677753-07-0 CAPLUS

CN Piperazine, 1-[[4-[2-[[4-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 677753-13-8 CAPLUS

CN Piperazine, 1-[[4-[2-[(4-chlorophenyl)amino]-4-pyrimidinyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 677753-14-9 CAPLUS

CN Piperazine, 1-[[4-[2-[(3,5-difluorophenyl)amino]-4-pyrimidinyl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

IT 677752-85-1P 677752-91-9P 677752-93-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and QSAR studies of series of potent and selective aminopyrimidine IKK2 inhibitors)

RN 677752-85-1 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[4-[2-[[4-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 677752-91-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[4-[2-[(4-chlorophenyl)amino]-4-pyrimidinyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

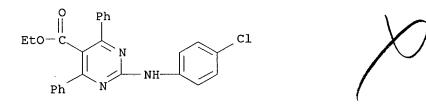
RN 677752-93-1 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[4-[2-[(3,5-difluorophenyl)amino]-4-pyrimidinyl]phenyl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

### 10/501,445

- L4 ANSWER 22 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2003:907999 CAPLUS
- DN 141:89052.
- TI Polymer-assisted synthesis of ethyl 2-amino-4,6-diarylpyrimidine-5-carboxylates
- AU Vanden Eynde, Jean Jacques; Labuche, Nadege; Van Haverbeke, Yves; Tietze,
- CS College of Pharmacy, Division of Basic Pharmaceutical Sciences, Xavier University of Louisiana, New Orleans, LX, 70125, USA
- SO ARKIVOC (Gainesville, FL, United States) (2003), (15), 22-28
  CODEN: AGFUAR
  URL: http://www.arkat-usa.org/ark/journal/2003/General\_Part(xv)/03-805B/805B.pdf
- PB Arkat USA Inc.
- DT Journal; (online computer file)
- LA English
- OS CASREACT 141:89052
- AB Et 2-amino-4,6-diarylpyrimidine-5-carboxylatesI [R1 = H; R2 = Ph, 4-ClC6H4, 4-MeOC6H4, n-Bu; R3 = H; R2R3 = (CH2)4, (CH2)2O(CH2)2; R1 = H, MeO, O2N; R2 = R3 = Me] have been synthesized in modest to good yields by a five-step procedure that involves building of the heterocyclic moiety on a solid support derived from Merrifield resin and final displacement with an amine.
- IT 714250-71-2P
  - RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of amino(diaryl)pyrimidinecarboxylates via substitution of Merrifield resin with thiourea followed by heterocyclization with arylidene(benzoyl)acetates followed by double oxidation and resin cleavage with amines)
- RN 714250-71-2 CAPLUS
- CN 5-Pyrimidinecarboxylic acid, 2-[(4-chlorophenyl)amino]-4,6-diphenyl-, ethyl ester (9CI) (CA INDEX NAME)



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 23 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
     2003:610266 CAPLUS
AN
DN
     139:164802
     Phenylpyrimidine amines and amides as IgE inhibitors and their
TΙ
     pharmaceutical compositions and therapeutic uses
     Bulusu, Murty; Ettmayer, Peter; Weigand, Klaus; Woisetschlaeger, Max
IN
     Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
PA
SO
     PCT Int. Appl., 39 pp.
     CODEN: PIXXD2
     Patent
DТ
     English
LΑ
FAN.CNT 1
     PATENT NO.
                         KIND
                                 DATE
                                             APPLICATION NO.
                                                                     DATE
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     WO 2003063871
                          A1
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PΙ
                                                                     20030131
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             LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SE, SG,
             SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW
         RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI,
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                                                                     20030131
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
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                                 20050429
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     CN 1622807
                          Α
                                 20050601
                                             CN 2003-802737
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                                             JP 2003-563561
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                                             US 2003-501445
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     NO 2004003610
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                                             NO 2004-3610
                          Α
                                                                     20040830
PRAI GB 2002-2381
                          Α
                                 20020201
     GB 2002-21953
                          Α
                                 20020920
     WO 2003-EP973
                                 20030131
                          W
     MARPAT 139:164802
OS
     Title amines I are disclosed [wherein: R1 = halo, halo(C1-4)alkyl; R2 = H,
AB
     halo, halo(C1-4)alkyl; R3 = halo, halo(C1-4)alkyl; R4 = H, C1-8 alkyl,
     hydroxy(C1-6)alkyl, various acyl groups, including formyl, (un)substituted
     alkanoyl, aroyl, carbamoyl, and oxycarbonyls]. I are useful as IgE
     biosynthesis inhibitors. Claimed uses include therapy of
     IgE-synthesis-mediated diseases, autoimmune diseases, gastrointestinal
     diseases, and chronic rejection of transplants. Targeted diseases include
     allergic asthma and other allergic and inflammatory diseases. Over 70
     invention compds. and/or salts were prepared For instance,
     3-chloroacetophenone was condensed with DMF di-Me acetal to give
     3-ClC6H4COCH: CHNMe2 (II). Addition reaction of 4-trifluoromethylaniline with
     cyanamide in aqueous solution in the presence of HCl gave N-[4-
     (trifluoromethyl)phenyl]guanidine, isolated as the carbonate (III).
     Cyclocondensation of II with III in n-BuOH at 120° gave invention
     compound IV [R4 = H]. Treatment of this with phospene and then
     MeN(CH2CH2OH)2 gave the derivative IV [R4 = COOCH2CH2N(Me)CH2CH2OH], isolated
     as the HCl salt. Compds. I (R4 \neq H) were less stable in human and
     murine plasma than compds. I (R4 = H) (no data), and may thus be
     considered to be prodrugs of the latter. The outcomes of several
     bioassays are also described (no data). I inhibit IgE production
     preferentially over IgG. I also inhibit IL-4 and anti-CD40 antibody
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mediated B-cell proliferation above the concns. needed to block IgE synthesis. I modulated DC cell surface markers, inhibiting the expression levels of CD86, HLA-Dr, CD83, and CD25. I also inhibited DC-mediated T-cell proliferation and cytokine production

574759-62-9P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]amine 574760-05-7P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-4-(methoxycarbonyl)butanamide 574760-06-8P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-5-(methoxycarbonyl)pentanamide 574760-10-4P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-4-carboxybutanamide

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; phenylpyrimidine amines as IgE inhibitors and their pharmaceutical compns. and therapeutic uses)

RN 574759-62-9 CAPLUS

IT

CN 2-Pyrimidinamine, 4-(3-chlorophenyl)-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574760-05-7 CAPLUS

CN Pentanoic acid, 5-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-5-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 574760-06-8 CAPLUS

CN

Hexanoic acid, 6-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

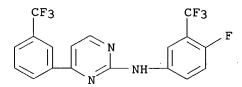
RN 574760-10-4 CAPLUS
CN Pentanoic acid, 5-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-

rentanoic acid, 5-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-5-oxo- (9CI) (CA INDEX NAME)

IT 574759-63-0P, N-[4-[3-(Trifluoromethyl)phenyl]pyrimidin-2-yl]-N-[4fluoro-3-(trifluoromethyl)phenyl]amine 574759-64-1P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-chloro-3-(trifluoromethyl)phenyl]amine 574759-65-2P, N-[4-[3-(Trifluoromethyl)phenyl]pyrimidin-2-yl]-N-[4-chloro-3-(trifluoromethyl)phenyl]amine 574759-66-3P, N-[4-[3-(Trifluoromethyl)phenyl]pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]amine 574759-67-4P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(3-Chlorophenyl)pyrimidin(trifluoromethyl)phenyl]acetamide 574759-68-5P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]propanam ide 574759-69-6P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-2-methylpropanamide 574759-70-9P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]benzamid e 574759-71-0P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-3-methylbutanamide 574759-72-1P,  $N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-\alpha$ oxobenzeneacetamide 574759-73-2P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-2,2-dimethylpropanamide 574759-74-3P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-<math>[4-(3-Chlorophenyl)pyrimidin-2-yl](trifluoromethyl)phenyl]cyclohexanecarboxamide 574759-75-4P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-3,4,5,6tetrahydro-2H-pyran-4-carboxamide 574759-76-5P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-2ethoxy-2-oxoacetamide 574759-77-6P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-2acetoxyacetamide 574759-78-7P, N-[4-(3-Chlorophenyl)pyrimidin-2yl]-N-[4-(trifluoromethyl)phenyl]-2-methoxy-2-oxoacetamide 574759-79-8P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-<math>[4-(3-Chlorophenyl)pyrimidin-2-yl](trifluoromethyl)phenyl]cyclopropanecarboxamide 574759-80-1P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-2-

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methoxyacetamide 574759-81-2P, (S)-N-[4-(3-1)]
 Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-2-
 acetoxypropanamide 574759-82-3P 574759-83-4P,
 [4-(3-Chlorophenyl)pyrimidin-2-yl][4-(trifluoromethyl)phenyl]carbamic acid
 3-aminopropyl ester hydrochloride 574759-84-5P,
 (S)-[4-(3-Chlorophenyl)pyrimidin-2-yl][4-(trifluoromethyl)phenyl]carbamic
acid 2-aminopropyl ester hydrochloride 574759-85-6P,
 [4-(3-Chlorophenyl)pyrimidin-2-yl][4-(trifluoromethyl)phenyl]carbamic acid
 2-[(2-hydroxyethyl)amino]ethyl ester hydrochloride 574759-86-7P,
 (S)-[4-(3-Chlorophenyl)pyrimidin-2-yl][4-(trifluoromethyl)phenyl]carbamic
 acid (pyrrolidin-2-yl)methyl ester hydrochloride 574759-87-8P,
 (S)-[4-(3-Chlorophenyl)pyrimidin-2-yl][4-(trifluoromethyl)phenyl]carbamic
 acid 2-aminoethyl ester hydrochloride 574759-88-9P,
 (S)-[4-(3-Chlorophenyl)pyrimidin-2-yl][4-(trifluoromethyl)phenyl]carbamic
 acid 2-amino-2-carboxyethyl ester hydrochloride 574759-89-0P
 574759-90-3P 574759-91-4P 574759-93-6P
 574759-94-7P, [4-(3-Chlorophenyl)pyrimidin-2-yl][4-
 (trifluoromethyl)phenyl]carbamic acid 2-[(2-hydroxyethyl)(methyl)amino]eth
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 hydrochloride 574759-98-1P, [4-(3-Chlorophenyl)pyrimidin-2-yl][4-
 (trifluoromethyl)phenyl]carbamic acid 3-(dimethylamino)propyl ester
 hydrochloride 574759-99-2P, [4-(3-Chlorophenyl)pyrimidin-2-yl][4-
 (trifluoromethyl)phenyl]carbamic acid 3-hydroxypropyl ester
 574760-00-2P, [4-(3-Chlorophenyl)pyrimidin-2-yl][4-
 (trifluoromethyl)phenyl]carbamic acid 2-(dimethylamino)ethyl ester
 hydrochloride 574760-01-3P, [4-(3-Chlorophenyl)pyrimidin-2-yl][4-
 (trifluoromethyl)phenyl]carbamic acid 2-[4-(2-hydroxyethyl)piperazin-1-
 yl]ethyl ester hydrochloride 574760-02-4P, [4-(3-
 Chlorophenyl)pyrimidin-2-yl][4-(trifluoromethyl)phenyl]carbamic acid
 2-(4-methylpiperazin-1-yl)ethyl ester 574760-03-5P,
 [4-(3-Chlorophenyl)pyrimidin-2-yl](methyl)[4-(trifluoromethyl)phenyl]amine
 574760-04-6P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-<math>[4-(3-Chlorophenyl)pyrimidin-2-yl]
 (trifluoromethyl)phenyl]-N', N'-dimethylurea 574760-07-9P,
 N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-3-
 (methoxycarbonyl) propanamide 574760-08-0P, N-[4-(3-
 Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-2-
 [(methoxycarbonyl)methoxy]acetamide 574760-09-1P,
 N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-2-(2-yl)-N-[4-(trifluoromethyl)phenyl]-2-(2-yl)-N-[4-(trifluoromethyl)phenyl]-2-(2-yl)-N-[4-(trifluoromethyl)phenyl]-2-(2-yl)-N-[4-(trifluoromethyl)phenyl]-2-(2-yl)-N-[4-(trifluoromethyl)phenyl]-2-(2-yl)-N-[4-(trifluoromethyl)phenyl]-2-(2-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromethyl)phenyl]-2-(4-yl)-N-[4-(trifluoromet
 methoxyethoxy) acetamide 574760-11-5P,
 N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-5-
 carboxypentanamide 574760-12-6P 574760-13-7P
 574760-14-8P 574760-15-9P 574760-16-0P
 574760-17-1P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-<math>[4-(3-Chlorophenyl)pyrimidin-2-yl]
 (trifluoromethyl)phenyl]-3-(diethylcarbamoyl)propanamide
 574760-18-2P, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-<math>[4-(3-Chlorophenyl)pyrimidin-2-yl]
 (trifluoromethyl)phenyl]-3-[N-[3-(dimethylamino)propyl]carbamoyl]propanami
 de 574760-19-3P 574760-20-6P 574760-21-7P
 574760-22-8P 574760-23-9P 574760-24-0P
 574760-25-1P 574760-26-2P 574760-27-3P,
 N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-4-(N,N-
 diethylcarbamoyl)butanamide 574760-28-4P, N-[4-(3-
 Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-4-[N-[3-
 (dimethylamino)propyl]carbamoyl]butanamide 574760-29-5P,
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N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-3-[[5-
(2-carboxyethoxy)pentyl]oxy]propanamide 574760-30-8P,
[4-(3-Chlorophenyl)pyrimidin-2-yl][4-(trifluoromethyl)phenyl]carbamic acid
3-[((S)-2-aminopropionyl)amino]propyl ester hydrochloride
574760-32-0P 574760-33-1P, [4-(3-Chlorophenyl)pyrimidin-
2-yl][4-(trifluoromethyl)phenyl]carbamic acid 2-[(2-
hydroxyethyl) (methyl) amino] ethyl ester 574760-34-2P,
[4-(3-Chlorophenyl)pyrimidin-2-yl](4-trifluoromethylphenyl)carbamic acid
2-[(2-hydroxyethyl)(methyl)amino]ethyl ester mesylate 574760-35-3P
, [4-(3-Chlorophenyl)pyrimidin-2-yl](4-trifluoromethylphenyl)carbamic acid
2-[(2-hydroxyethyl)(methyl)amino]ethyl ester sulfate 574760-36-4P
, [4-(3-Chlorophenyl)pyrimidin-2-yl](4-trifluoromethylphenyl)carbamic acid
2-[(2-hydroxyethyl)(methyl)amino]ethyl ester tartrate 574760-37-5P
, [4-(3-Chlorophenyl)pyrimidin-2-yl](4-trifluoromethylphenyl)carbamic acid
2-[(2-hydroxyethyl)(methyl)amino]ethyl ester tosylate 574760-38-6P
, [4-(3-Chlorophenyl)pyrimidin-2-yl](4-trifluoromethylphenyl)carbamic acid
2-[(2-hydroxyethyl)(methyl)amino]ethyl ester besylate 574760-39-7P
, N-[4-(3-Chlorophenyl)pyrimidin-2-yl]-N-[4-(trifluoromethyl)phenyl]-4-
carboxybutanamide calcium salt
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (drug candidate; phenylpyrimidine amines as IgE inhibitors and their
  pharmaceutical compns. and therapeutic uses)
574759-63-0 CAPLUS
2-Pyrimidinamine, N-[4-fluoro-3-(trifluoromethyl)phenyl]-4-[3-
(trifluoromethyl)phenyl] - (9CI) (CA INDEX NAME)
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RN

CN

RN 574759-64-1 CAPLUS
CN 2-Pyrimidinamine, 4-(3-chlorophenyl)-N-[4-chloro-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-66-3 CAPLUS

CN 2-Pyrimidinamine, 4-[3-(trifluoromethyl)phenyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-67-4 CAPLUS

CN Acetamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-68-5 CAPLUS

CN Propanamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-69-6 CAPLUS

CN Propanamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-2-methyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-70-9 CAPLUS

CN Benzamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-71-0 CAPLUS

CN Butanamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-3-methyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-72-1 CAPLUS

CN Benzeneacetamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]- $\alpha$ -oxo-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-73-2 CAPLUS

CN Propanamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-2,2-dimethyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-74-3 CAPLUS

CN Cyclohexanecarboxamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-75-4 CAPLUS

CN 2H-Pyran-4-carboxamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]tetrahydro-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-76-5 CAPLUS

CN Acetic acid, [[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 574759-77-6 CAPLUS

CN Acetamide, 2-(acetyloxy)-N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-78-7 CAPLUS

CN Acetic acid, [[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 574759-79-8 CAPLUS

CN Cyclopropanecarboxamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-80-1 CAPLUS

CN Acetamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-2-methoxy-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574759-81-2 CAPLUS

CN Propanamide, 2-(acetyloxy)-N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N-[4-(trifluoromethyl)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 574759-82-3 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 3-[[(2S)-2-amino-1-oxopropyl]amino]propyl ester (9CI) (CA INDEX NAME)

RN 574759-83-4 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 3-aminopropyl ester, hydrochloride (9CI) (CA INDEX NAME)

## ●x HCl

RN 574759-84-5 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, (2S)-2-aminopropyl ester, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## ●x HCl

RN 574759-85-6 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[(2-hydroxyethyl)amino]ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 574759-86-7 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, (2S)-2-pyrrolidinylmethyl ester, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●x HCl

RN 574759-87-8 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-aminoethyl ester, hydrochloride (9CI) (CA INDEX NAME)

RN 574759-88-9 CAPLUS

CN L-Serine, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]carbamate (ester), hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## ●x HCl

RN 574759-89-0 CAPLUS

CN D-Alanine, 2-[[[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]carbonyl]oxy]ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

RN 574759-90-3 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[[(2R)-2-amino-1-oxopropyl]amino]ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### ●x HCl

RN 574759-91-4 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[[(2R,3R)-2-amino-3-hydroxy-1-oxobutyl]amino]ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

RN 574759-93-6 CAPLUS

CN L-Alanine, 3-[[[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]carbonyl]oxy]propyl ester, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 574759-92-5

CMF C24 H22 C1 F3 N4 O4

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 574759-94-7 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[(2-hydroxyethyl)methylamino]ethyl ester,

hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 574759-95-8 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 574759-96-9 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-(4-morpholinyl)ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
CF3 \\
O \\
N \\
CH_2 - CH_2 - O - C \\
N \\
N
\end{array}$$
C1

●x HCl

RN 574759-97-0 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-(1-pyrrolidinyl)ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

RN 574759-98-1 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 3-(dimethylamino)propyl ester, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 574759-99-2 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 3-hydroxypropyl ester (9CI) (CA INDEX NAME)

RN 574760-00-2 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-(dimethylamino)ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

•x HCl

RN 574760-01-3 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[4-(2-hydroxyethyl)-1-piperazinyl]ethyl ester, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CF3} \\ \text{N} \\ \text{CO} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CO} \\ \text{C$$

●x HCl

RN 574760-02-4 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-(4-methyl-1-piperazinyl)ethyl ester (9CI) (CA INDEX NAME)

RN 574760-03-5 CAPLUS

CN 2-Pyrimidinamine, 4-(3-chlorophenyl)-N-methyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574760-04-6 CAPLUS

CN Urea, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N',N'-dimethyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574760-07-9 CAPLUS

CN Butanoic acid, 4-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \circ \\ & \subset \mathsf{CH_2-CH_2-C-OMe} \\ & & & \mathsf{CF_3} \end{array}$$

RN 574760-08-0 CAPLUS

CN Acetic acid, [2-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-2-oxoethoxy]-, methyl ester (9CI) (CA

INDEX NAME)

RN 574760-09-1 CAPLUS

CN Acetamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-2-(2-methoxyethoxy)-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574760-11-5 CAPLUS

CN Hexanoic acid, 6-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-6-oxo-(9CI) (CA INDEX NAME)

RN 574760-12-6 CAPLUS

CN L-Alanine, N-[4-[[4-(3-chlorophenyl)-2-pyrimidinyl]][4-(trifluoromethyl)phenyl]amino]-1,4-dioxobutyl]- (9CI) (CA INDEX NAME)

RN 574760-13-7 CAPLUS

CN L-Alanine, N-[5-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-1,5-dioxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 574760-14-8 CAPLUS

CN L-Alanine, N-[[2-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-2-oxoethoxy]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 574760-15-9 CAPLUS

CN L-Alanine, N-[4-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-1,4-dioxobutyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 574760-16-0 CAPLUS

CN L-Phenylalanine, N-[5-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-1,5-dioxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 574760-17-1 CAPLUS

CN Butanediamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N',N'-diethyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574760-18-2 CAPLUS

CN Butanediamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N'-[3-(dimethylamino)propyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574760-19-3 CAPLUS

CN L-Glutamic acid, N-[4-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-1,4-dioxobutyl]-, 1-methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 574760-20-6 CAPLUS '

CN L-Phenylalanine, N-[4-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-1,4-dioxobutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 574760-21-7 CAPLUS

CN L-Glutamic acid, N-[4-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-1,4-dioxobutyl]-, dimethyl ester (9CI) (CA INDEX NAME)

RN 574760-22-8 CAPLUS

CN L-Glutamic acid, N-[5-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-1,5-dioxopentyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 574760-23-9 CAPLUS

CN L-Glutamic acid, N-[5-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-1,5-dioxopentyl]-, 5-methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 574760-24-0 CAPLUS

CN L-Alanine, N-[5-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-1,5-dioxopentyl]-, methyl ester (9CI) (CAINDEX NAME)

RN 574760-25-1 CAPLUS

CN L-Alanine, N-[[2-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-2-oxoethoxy]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 574760-26-2 CAPLUS

CN L-Lysine, N2-acetyl-N6-[4-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-1,4-dioxobutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 574760-27-3 CAPLUS

CN Pentanediamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N',N'-diethyl-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574760-28-4 CAPLUS

CN Pentanediamide, N-[4-(3-chlorophenyl)-2-pyrimidinyl]-N'-[3-(dimethylamino)propyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 574760-29-5 CAPLUS

CN Propanoic acid, 3-[[5-[3-[[4-(3-chlorophenyl)-2-pyrimidinyl]][4-(trifluoromethyl)phenyl]amino]-3-oxopropoxy]pentyl]oxy]- (9CI) (CA INDEX NAME)

RN 574760-30-8 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 3-[[(2S)-2-amino-1-oxopropyl]amino]propyl ester, hydrochloride (9CI) (CA INDEX NAME)

RN 574760-32-0 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[[(2R)-2-amino-1-oxopropyl]amino]ethyl ester, benzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 574760-31-9

CMF C23 H21 C1 F3 N5 O3

Absolute stereochemistry.

CM 2

CRN 98-11-3 CMF C6 H6 O3 S

RN 574760-33-1 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-

(trifluoromethyl)phenyl]-, 2-[(2-hydroxyethyl)methylamino]ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & Me \\ \parallel & \parallel \\ C-O-CH_2-CH_2-N-CH_2-CH_2-OH \\ \hline \\ CF_3 \\ \end{array}$$

RN 574760-34-2 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[(2-hydroxyethyl)methylamino]ethyl ester, methanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 574760-33-1 CMF C23 H22 Cl F3 N4 O3

CM 2

CRN 75-75-2 CMF C H4 O3 S

RN 574760-35-3 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[(2-hydroxyethyl)methylamino]ethyl ester, sulfate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 574760-33-1 CMF C23 H22 C1 F3 N4 O3

CM 2

CRN 7664-93-9 CMF H2 O4 S

RN 574760-36-4 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[(2-hydroxyethyl)methylamino]ethyl ester, (2R,3R)-2,3-dihydroxybutanedioate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 574760-33-1 CMF C23 H22 Cl F3 N4 O3

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

RN 574760-37-5 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[(2-hydroxyethyl)methylamino]ethyl ester, 4-methylbenzenesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 574760-33-1

CMF C23 H22 C1 F3 N4 O3

$$\begin{array}{c|c} O & Me \\ \parallel & \parallel \\ C-O-CH_2-CH_2-N-CH_2-CH_2-OH \\ \hline \\ CF_3 \\ \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 574760-38-6 CAPLUS

CN Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 2-[(2-hydroxyethyl)methylamino]ethyl ester, benzenesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 574760-33-1

CMF C23 H22 C1 F3 N4 O3

$$\begin{array}{c|c} O & Me \\ \parallel & \parallel \\ C-O-CH_2-CH_2-N-CH_2-CH_2-OH \\ \hline \\ CF_3 \\ \end{array}$$

CM 2

CRN 98-11-3 CMF C6 H6 O3 S

RN 574760-39-7 CAPLUS

CN Pentanoic acid, 5-[[4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]amino]-5-oxo-, calcium salt (9CI) (CA INDEX NAME)

## ●1/2 Ca

RN 574760-41-1 CAPLUS CN Carbamic acid, [4-(

Carbamic acid, [4-(3-chlorophenyl)-2-pyrimidinyl][4-(trifluoromethyl)phenyl]-, 3-[[(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxopropyl]amino]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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T.4
     ANSWER 24 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
ΑN
     2002:777933 CAPLUS
DN
     137:294969
ΤI
     4-Aryl-substituted 2-pyrimidinamines and 2-pyridinamines, useful as
     inhibitors of c-Jun N-terminal kinases (JNK) and other protein kinases
IN
     Bethiel, Randy; Cochran, John; Moon, Young-Choon; Nanthakumar, Susanthini
     Vertex Pharmaceuticals Incorporated, USA
PΑ
SO
     PCT Int. Appl., 115 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LΑ
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os
     MARPAT 137:294969
     The invention provides compds. of formula I and II, and their
AΒ
     pharmaceutically acceptable derivs. [wherein: W = N, CH; R1, R2, R3 = halo,
     QR, QnCN, QnNO2, QnAr2; or R1R2, R2R3 = 4- to 8-membered (un)saturated ring
     with 0-3 N/O/S atoms; n = 0 or 1; Q = C1-4 alkylidene with one CH2
     optionally replaced by O, S, NR, NRCO, CO, CO2, CONR, SO2, SO2NR, NRSO2NR,
     etc.; R = H, (un)substituted aliphatic; or NRR = 3- to 7-membered (un)saturated
     ring with 1-2 addnl. N/O/S atoms; R4 = Ar1, TAr2, TnAr3; T = C1-2
     alkylidene with optional replacement of a CH2 as above; Ar1 =
     (un) substituted 5- to 6-membered mono- or bicyclic (un) saturated ring system;
     Ar2 = (un)  substituted 5- to 6-membered (un) saturated monocyclic ring with 0-3
     N/O/S atoms, or (un)substituted 8- to 10-membered (un)saturated bicyclic ring
     with 0-5 \text{ N/O/S} atoms; Ar3 = 6-membered aryl with 0-2 \text{ N} atoms and
     substituted with certain groups; with provisos and exclusions].
     compds. are inhibitors of protein kinases, particularly JNK, a mammalian
     protein kinase involved in cell proliferation, cell death and response to
     extracellular stimuli. Furthermore, they are inhibitors of Src-family
     kinases, especially Src and Lck kinases. The compds. are also inhibitors of
     GSK3 and CDK2 kinases. The invention also relates to methods for
     producing the compds. Also provided are pharmaceutical compns. comprising
     I or II, and methods of utilizing those compns. in the treatment and
     prevention of various disorders. Three tables of approx. 240 compds. were
     prepared and claimed., and most were tested against at least one of the five
     mentioned kinases. For instance, 3,4-dihydroxy-5-methoxybenzaldehyde was
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cyclized with 1,2-dibromoethane to give a benzodioxane derivative, followed by

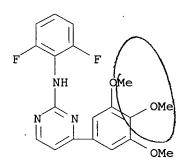
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elaboration of the formyl group to Me2NCH:CO- in 3 steps. Cyclization
    of the resultant enaminone with 3-chlorophenylquanidine gave title compound
     III. This compound inhibited cloned human JNK3 protein in vitro with Ki <
     0.1 \, \mu M.
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     468084-22-2P, 4-(3,4,5-Trimethoxyphenyl)-N-(2-fluorophenyl)-2-
    pyrimidinamine 468084-23-3P 468084-29-9P,
     4-(3,4,5-Trimethoxyphenyl)-N-(2,3-difluorophenyl)-2-pyrimidinamine
     468084-32-4P, 4-(3,4,5-Trimethoxyphenyl)-N-(3-chlorophenyl)-2-
    pyrimidinamine 468084-33-5P, 4-(3,4,5-Trimethoxyphenyl)-N-(3-
     (trifluoromethyl)phenyl)-2-pyrimidinamine 468084-36-8P,
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     468084-37-9P, 4-(3,4,5-Trimethoxypheny1)-N-(3,5-dichloropheny1)-2-
    pyrimidinamine 468084-53-9P, 4-(3,4,5-Trimethoxyphenyl)-N-(3-
     chloro-4-methoxyphenyl)-2-pyrimidinamine 468084-58-4P,
     4-(3,5-Dimethoxy-4-(2-morpholinoethoxy)phenyl)-N-(3-chlorophenyl)-2-
    pyrimidinamine 468084-59-5P, 4-(4-Ethoxy-3,5-dimethoxyphenyl)-N-
     (3-chlorophenyl)-2-pyrimidinamine 468084-60-8P,
     4-(3,5-Dichloro-4-methoxyphenyl)-N-(3-chlorophenyl)-2-pyrimidinamine
     468084-61-9P, 4-(3,5-Dimethyl-4-methoxyphenyl)-N-(3-chlorophenyl)-
     2-pyrimidinamine 468084-62-0P, 4-(3,5-Dibromo-4-methoxyphenyl)-N-
     (3-chlorophenyl)-2-pyrimidinamine 468084-63-1P,
     4-(3,5-Dimethoxy-4-(2-morpholinoethoxy)phenyl)-N-(3-fluorophenyl)-2-
    pyrimidinamine 468084-64-2P, 4-(4-Ethoxy-3,5-dimethoxyphenyl)-N-
     (3-fluorophenyl)-2-pyrimidinamine 468084-65-3P,
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     468084-66-4P, 4-(3,5-Dimethyl-4-methoxyphenyl)-N-(3-fluorophenyl)-
     2-pyrimidinamine 468084-67-5P, 4-(3,5-Dibromo-4-methoxyphenyl)-N-
     (3-fluorophenyl)-2-pyrimidinamine 468084-77-7P,
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     468085-90-7P, 4-(2,3,4-Trimethoxyphenyl)-N-(3-fluorophenyl)-2-
     pyrimidinamine 468085-92-9P, 4-(2,3,4-Trimethoxyphenyl)-N-(4-
     fluorophenyl)-2-pyrimidinamine 468085-93-0P,
     4-(2,3,4-Trimethoxyphenyl)-N-(4-chlorophenyl)-2-pyrimidinamine
     468085-94-1P, 4-(2,3,4-Trimethoxyphenyl)-N-(3,4-difluorophenyl)-2-
     pyrimidinamine 468086-56-8P, 4-(2,3,4-Trimethoxyphenyl)-N-(3'-
     chloro-4-fluoro-1,1'-biphenyl-3-yl)-2-pyrimidinamine
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (drug candidate; preparation of phenyl-substituted pyridinamines and
       pyrimidinamines as inhibitors of c-Jun N-terminal kinases (JNK) and
       other protein kinases)
     468084-18-6 CAPLUS
RN
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2-Pyrimidinamine, N-(4-chlorophenyl)-4-(3,4,5-trimethoxyphenyl)- (9CI)

CN

(CA INDEX NAME)

RN 468084-19-7 CAPLUS
CN 2-Pyrimidinamine, N-(2,6-difluorophenyl)-4-(3,4,5-trimethoxyphenyl)- (9CI)
(CA INDEX NAME)



RN 468084-20-0 CAPLUS
CN 2-Pyrimidinamine, N-(4-fluorophenyl)-4-(3,4,5-trimethoxyphenyl)- (9CI)
(CA INDEX NAME)

RN 468084-22-2 CAPLUS
CN 2-Pyrimidinamine, N-(2-fluorophenyl)-4-(3,4,5-trimethoxyphenyl)- (9CI)
(CA INDEX NAME)

RN 468084-23-3 CAPLUS

CN 2-Pyrimidinamine, N-(3-fluorophenyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 468084-29-9 CAPLUS

CN 2-Pyrimidinamine, N-(2,3-difluorophenyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 468084-32-4 CAPLUS

CN 2-Pyrimidinamine, N-(3-chlorophenyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 468084-33-5 CAPLUS

CN 2-Pyrimidinamine, N-[3-(trifluoromethyl)phenyl]-4-(3,4,5-trimethoxyphenyl)-(9CI) (CA INDEX NAME)

RN 468084-36-8 CAPLUS

CN 2-Pyrimidinamine, N-(3,4,5-trifluorophenyl)-4-(3,4,5-trimethoxyphenyl)-(9CI) (CA INDEX NAME)

RN 468084-37-9 CAPLUS

CN 2-Pyrimidinamine, N-(3,5-dichlorophenyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 468084-53-9 CAPLUS

CN 2-Pyrimidinamine, N-(3-chloro-4-methoxyphenyl)-4-(3,4,5-trimethoxyphenyl)-(9CI) (CA INDEX NAME)

RN 468084-58-4 CAPLUS

CN 2-Pyrimidinamine, N-(3-chlorophenyl)-4-[3,5-dimethoxy-4-[2-(4-morpholinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

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RN 468084-59-5 CAPLUS

CN 2-Pyrimidinamine, N-(3-chlorophenyl)-4-(4-ethoxy-3,5-dimethoxyphenyl)-(9CI) (CA INDEX NAME)

RN 468084-60-8 CAPLUS

CN 2-Pyrimidinamine, N-(3-chlorophenyl)-4-(3,5-dichloro-4-methoxyphenyl)-(9CI) (CA INDEX NAME)

RN 468084-61-9 CAPLUS

CN 2-Pyrimidinamine, N-(3-chlorophenyl)-4-(4-methoxy-3,5-dimethylphenyl)-(9CI) (CA INDEX NAME)

RN 468084-62-0 CAPLUS

CN 2-Pyrimidinamine, N-(3-chlorophenyl)-4-(3,5-dibromo-4-methoxyphenyl)(9CI) (CA INDEX NAME)

RN 468084-63-1 CAPLUS

CN 2-Pyrimidinamine, 4-[3,5-dimethoxy-4-[2-(4-morpholinyl)ethoxy]phenyl]-N-(3-fluorophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \hline \\ O & & \\ \hline \\ O & & \\ \hline \\ O & & \\ \end{array}$$

RN 468084-64-2 CAPLUS

CN 2-Pyrimidinamine, 4-(4-ethoxy-3,5-dimethoxyphenyl)-N-(3-fluorophenyl)-(9CI) (CA INDEX NAME)

RN 468084-65-3 CAPLUS

CN 2-Pyrimidinamine, 4-(3,5-dichloro-4-methoxyphenyl)-N-(3-fluorophenyl)-(9CI) (CA INDEX NAME)

RN 468084-66-4 CAPLUS

CN 2-Pyrimidinamine, N-(3-fluorophenyl)-4-(4-methoxy-3,5-dimethylphenyl)-(9CI) (CA INDEX NAME)

RN 468084-67-5 CAPLUS

CN 2-Pyrimidinamine, 4-(3,5-dibromo-4-methoxyphenyl)-N-(3-fluorophenyl)-(9CI) (CA INDEX NAME)

RN 468084-77-7 CAPLUS

CN 2-Pyrimidinamine, N-(3-bromophenyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 468085-90-7 CAPLUS
CN 2-Pyrimidinamine, N-(3-fluorophenyl)-4-(2,3,4-trimethoxyphenyl)- (9CI)
(CA INDEX NAME)

RN 468085-92-9 CAPLUS
CN 2-Pyrimidinamine, N-(4-fluorophenyl)-4-(2,3,4-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 468085-93-0 CAPLUS
CN 2-Pyrimidinamine, N-(4-chlorophenyl)-4-(2,3,4-trimethoxyphenyl)- (9CI)
(CA INDEX NAME)

RN 468085-94-1 CAPLUS
CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-(2,3,4-trimethoxyphenyl)- (9CI)
(CA INDEX NAME)

RN 468086-56-8 CAPLUS
CN 2-Pyrimidinamine, N-(3'-chloro-4-fluoro[1,1'-biphenyl]-3-yl)-4-(2,3,4-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4
     ANSWER 25 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
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     2002:615605 CAPLUS
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     137:169539
     Preparation of 3-(4-pyrimidinylamino)-1H-pyrazoles as protein kinase
ΤI
     inhibitors, especially of Aurora-2 and GSK-3, for treatment of cancer,
     diabetes, and Alzheimer's disease
IN
     Bebbington, David; Charrier, Jean-Damien; Golec, Julian M. C.; Miller,
     Andrew; Knegtel, Ronald
     Vertex Pharmaceuticals Incorporated, USA
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     PCT Int. Appl., 335 pp.
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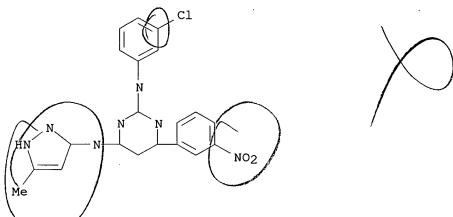
AΒ 285 Title compds. I [wherein Z1 = N or CR8; Z2 = N or CH; and at least 1 of Z1 and Z2 = N; Rx and Ry = independently TR3 or LZR3; or C2RxRy = (un) substituted fused (hetero) cycle; Q = NR4, O, S, C(R6')2, 1,2-cyclo(prop/but)anediyl, or 1,3-cyclobutanediyl; R1 = TD; D = (un) substituted mono- or bicyclic (hetero) aryl, heterocyclyl, or carbocyclyl; T = a bond or alkylidene chain (un)interrupted by O, S, NR4, CO, CONH, NHCO, SO2, SO2NH, NHSO2, CO2, OCO, OCONH, or NHCO2, with provisos; Z = alkylidene chain; L = O, S, SO, SO2, NR6SO2, SO2NR6, NR6, NR6CO, NR6CO2, NR6CONR6, NR6SO2NR6, NR6NR6, OCONR6, or W; R2 and R2a = independently R, TWR6, or C2R2R2a = (un)substituted fused (hetero)cycle; R3 = R, halo, OR, COR, CO2R, CO(CH2)0-1COR, NO2, CN, SO0-2R, N(R4)2, carbamoyl, sulfamoyl, OCOR, acylamino, hydrazino, ureido, etc.; R = independently H or (un) substituted aliphatic, (hetero) aryl, or heterocyclyl; R4 = independently R7, COR7, carboxy, CON(R7)2, or SO2R7; W = CO, CO2, CONR6, C(R6)20, C(R6)2S00-2, C(R6)2S02NR6, C(R6)2NR6, C(R6)2NR6C0, C(R6) 2NR6CO2, CR6:NNR6, CR6:NO, C(R6) 2NR6NR6, C(R6) 2NR6SO2NR6, or C(R6)2NR6CONR6; R6, R6', R7 = independently H or aliphatic; or N(R6)2 or N(R7)2 = independently heterocyclyl or heteroaryl; or C(R6')2 = carbocycle; R8 = R, halo, OR, COR, CO2R, COCOR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2(R4)2, OCOR, NR4COR, NR4CO2(aliphatic), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2] were prepared However, the claims pertain only to 3-(2-amino-4-pyrimidinylamino)-1Hpyrazoles, i.e. Z1 = Z2 = N, and Q = NH. I are protein kinase inhibitors, especially of Aurora-2 and GSK-3. For example, the (pyrazolylamino)quinazoline II was refluxed with thiophenol in t-BuOH to give III. In bioassays, I. inhibited the following kinases with Ki values reported < 20 μM: GSK-3 $\beta$  (232 compds.), AURORA-2 (227 compds.), CDK-2 (13 compds.), ERK2 (8 compds.), AKT (10 compds.), and Human Src kinase (183 compds.). I are useful for the treatment of diseases associated with protein kinases, such as diabetes, cancer, and Alzheimer's disease (no data). IT 438205-79-9P 438205-80-2P 438205-86-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(protein kinase inhibitor; preparation of (pyrimidinylamino)pyrazoles as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 438205-79-9 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-(5-methyl-1H-pyrazol-3-yl)-6-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 438205-80-2 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-(5-methyl-1H-pyrazol-3-yl)-6-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 438205-86-8 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-[5-(1,1-dimethylethyl)-1H-pyrazol-3-yl]-6-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

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ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 26 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
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OS MARPAT 137:109292

ΑB Title compds. I [wherein Z1 = N or CR8; Z2 = N or CH; and at least 1 of Z1 and Z2 = N; Rx and Ry = independently TR3 or LZR3; or C2RxRy = (un) substituted fused (hetero) cycle; Q = NR4, O, S, C(6a)2, 1,2-cyclo(prop/but)anediyl, or 1,3-cyclobutanediyl; R1 = TD; D = (un) substituted mono- or bicyclic (hetero) aryl, heterocyclyl, or carbocyclyl; T = a bond or alkylidene chain (un)interrupted by O, S, NR4, CO, CONH, NHCO, SO2, SO2NH, NHSO2, CO2, OCO, OCONH, or NHCO2, with provisos; Z = alkylidene chain; L = O, S, SO, SO2, NR6SO2, SO2NR6, NR6, NR6CO, NR6CO2, NR6CONR6, NR6SO2NR6, NR6NR6, OCONR6, or W; R2 and R2a = independently R, TWR6, or C2R2R2a = (un)substituted fused (hetero)cycle; R3 = R, halo, OR, COR, CO2R, CO(CH2)0-1COR, NO2, CN, SO0-2R, N(R4)2, carbamoyl, sulfamoyl, OCOR, acylamino, hydrazino, ureido, etc.; R = independently H or (un) substituted aliphatic, (hetero) aryl, or heterocyclyl; R4 = independently R7, COR7, carboxy, CON(R7)2, or SO2R7; W = CO, CO2,CONR6, C(R6)20, C(R6)2S00-2, C(R6)2S02NR6, C(R6)2NR6, C(R6)2NR6CO, C(R6)2NR6CO2, CR6:NNR6, CR6:NO, C(R6)2NR6NR6, C(R6)2NR6SO2NR6, or C(R6)2NR6CONR6; R6, R6a, R7 = independently H or aliphatic; or N(R6)2 or N(R7)2 = independently heterocyclyl or heteroaryl; or C(R6a)2 =carbocycle; R8 = R, halo, OR, COR, CO2R, COCOR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2(R4)2, OCOR, NR4COR, NR4CO2(aliphatic), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2] were prepared I are protein kinase inhibitors, especially of Aurora-2 and GSK-3. For example, the (pyrazolylamino)quinazoline II was refluxed with thiophenol in t-BuOH to give III. In bioassays, I inhibited the following kinases with Ki values reported < 20  $\mu$ M: GSK-3 $\beta$  (232 compds.), AURORA-2 (227 compds.), CDK-2 (13 compds.), ERK2 (8 compds.), AKT (10 compds.), and Human Src kinase (183 compds.). I are useful for the treatment of diseases associated with protein kinases, such as diabetes, cancer, and Alzheimer's disease (no data).

IT 438205-79-9P 438205-80-2P 438205-86-8P 438205-87-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(protein kinase inhibitor; preparation of (pyrimidinylamino)pyrazoles as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 438205-79-9 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-(5-methyl-1H-pyrazol-3-yl)-6-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 438205-80-2 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-(5-methyl-1H-pyrazol-3-yl)-6-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

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RN 438205-86-8 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-[5-(1,1-dimethylethyl)-1H-pyrazol-3-yl]-6-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 438205-87-9 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-6-(3-nitrophenyl)-N4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

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US 2003004164

US 20030022885

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US 2001-34019

US 6727251

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US 2003-624800

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     Z2 = N; Rb, Rc = TR3, LZR3; C2RbRc = (un)substituted fused (hetero)cycle;
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     = H, alkyl; or N(R6)2 or N(R7)2 = heterocyclyl, heteroaryl] were prepared
     For example, the (pyrazolylamino)quinazoline II was refluxed with
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     following kinases with Ki values reported < 20 \muM: GSK-3\beta (232
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IT
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NO 2003002704
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US 2004224944
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US 7008948
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US 2004116454
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US 2004157893
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US 2004132781
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US 7087603
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US 2004167141
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JP 2005097322
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AU 2006201229
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     AU 2006201391
                           A1
                                 20060427
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PRAI US 2000-257887P
                           Р
                                 20001221
                           Ρ
     US 2001-286949P
                                 20010427
                           Р
     US 2000-232795P
                                 20000915
     AU 2001-90944
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                                 20010914
     AU 2001-91013
                           A3
                                 20010914
     AU 2001-94558
                           Α3
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     AU 2001-96871
                           Α3
                                 20010914
     AU 2001-96875
                           A3
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     EP 2001-971082
                           A3
                                 20010914
     US 2001-952671
                           А3
                                 20010914
     US 2001-955601
                           Α3
                                 20010914
     EP 2001-273861
                           Α
                                 20011219
     EP 2001-994323
                           Α3
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     JP 2002-557938
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                                 20011219
     US 2001-26966
                           A1
                                 20011219
     WO 2001-US49139
                           W
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     WO 2001-US49140
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     WO 2001-US50312
                           W
                                 20011219
     US 2001-34019
                           ΑЗ.
                                 20011220
     US 2001-34683
                           A1
                                 20011220
```

OS MARPAT 137:47221

AΒ

Title compds. I [wherein Z1 = N or CR8; Z2 = N or CH; and at least 1 of Z1 and Z2 = N; Rx and Ry = independently TR3 or LZR3; or C2RxRy = (un) substituted fused (hetero) cycle; Q = NR4, O, S, C(6a)2, 1,2-cyclo(prop/but)anediyl, or 1,3-cyclobutanediyl; R1 = TD; D = (un) substituted mono- or bicyclic (hetero) aryl, heterocyclyl, or carbocyclyl; T = a bond or alkylidene chain (un)interrupted by O, S, NR4, CO, CONH, NHCO, SO2, SO2NH, NHSO2, CO2, OCO, OCONH, or NHCO2, with provisos; Z = alkylidene chain; L = O, S, SO, SO2, NR6SO2, SO2NR6, NR6, NR6CO, NR6CO2, NR6CONR6, NR6SO2NR6, NR6NR6, OCONR6, or W; R2 and R2a = independently R, TWR6, or C2R2R2a = (un)substituted fused (hetero)cycle; R3 = R, halo, OR, COR, CO2R, CO(CH2)0-1COR, NO2, CN, SO0-2R, N(R4)2, carbamoyl, sulfamoyl, OCOR, acylamino, hydrazino, ureido, etc.; R = independently H or (un) substituted aliphatic, (hetero) aryl, or heterocyclyl; R4 = independently R7, COR7, carboxy, CON(R7)2, or SO2R7; W = CO, CO2,CONR6, C(R6)2O, C(R6)2SOO-2, C(R6)2SO2NR6, C(R6)2NR6, C(R6)2NR6CO, C(R6)2NR6CO2, CR6:NNR6, CR6:NO, C(R6)2NR6NR6, C(R6)2NR6SO2NR6, or C(R6) 2NR6CONR6; R6, R6a, R7 = independently H or aliphatic; or N(R6) 2 or N(R7)2 = independently heterocyclyl or heteroaryl; or C(R6a)2 = carbocycle; R8 = R, halo, OR, COR, CO2R, COCOR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2(R4)2, OCOR, NR4COR, NR4CO2(aliphatic), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2] were prepared I are protein kinase inhibitors, especially of Aurora-2 and GSK-3. For example, the (pyrazolylamino)quinazoline II was refluxed with thiophenol in t-BuOH to give III. In bioassays, I inhibited the following kinases with Ki values reported < 20  $\mu$ M: GSK-3 $\beta$  (232 compds.), AURORA-2 (227 compds.), CDK-2 (13 compds.), ERK2 (8 compds.), AKT (10 compds.), and Human Src kinase (183 compds.). I are useful for the treatment of diseases associated with protein kinases, such as diabetes, cancer, and Alzheimer's disease (no data).

IT 438205-79-9P 438205-80-2P 438205-86-8P

438205-87-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(protein kinase inhibitor; preparation of (pyrimidinylamino)pyrazoles as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 438205-79-9 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-(5-methyl-1H-pyrazol-3-yl)-6-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 438205-80-2 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-(5-methyl-1H-pyrazol-3-yl)-6-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 438205-86-8 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-N4-[5-(1,1-dimethylethyl)-1H-pyrazol-3-yl]-6-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 438205-87-9 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chlorophenyl)-6-(3-nitrophenyl)-N4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

## 10/501,445

Same of 33

L4 ANSWER 29 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:772132 CAPLUS

DN 135:303909

TI Preparation of aryl-substituted pyrimidines as insecticidal and acaricidal agents

IN Wood, William Wakefield; Fleming, Linda; Cuccia, Salvatore John

PA American Cyanamid Company, USA

SO U.S., 11 pp. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

FAN.CNT Z			•	
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6306866	B1	20011023	US 1998-36490	19980306
US 6153619	Α	20001128	US 1999-273942	19990322
US 2002045634	A1	20020418	US 2000-725376	20001129
US 6440984	B2	20020827	•	
PRAI US 1998-36490	A3	19980306		

OS MARPAT 135:303909

AB The title compds. [I; R1, R2 = H, halo, alkyl, etc.; A = substituted Ph; B = substituted Ph; one of Y and Z = N and the other = CR2; X = O, NR; R = H, alkyl], useful for the control of insect and acarid pests (biol. data given), were prepared E.g., a 2-step synthesis of I [Y = N; Z = CH; R1 = H; X = O; A = 3-F3CC6H4; B = 3,4-C12C6H3] was presented.

IT 309255-89-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of aryl-substituted pyrimidines as insecticidal and acaricidal agents)

RN 309255-89-8 CAPLUS

CN 2-Pyrimidinamine, N,4-bis[4-fluoro-3-(trifluoromethyl)phenyl]-N-methyl-(9CI) (CA INDEX NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 30 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
     2001:730738 CAPLUS
AN
DN
     135:288789
TI
     2-Substituted 4-heteroaryl-pyrimidines with activity as inhibitors of
     cyclin-dependent kinases and their preparation and use in the treatment of
     proliferative disorders
IN
     Fischer, Peter Martin; Wang, Shudong
PA
     Cyclacel Limited, UK
SO
     PCT Int. Appl., 95 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                           KIND .
                                   DATE
                                                APPLICATION NO.
                                                                          DATE
                                   _____
                                                ______
     WO 2001072745
                                   20011004
                                                WO 2001-GB1423
                                                                          20010,828
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              RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,
              VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
              DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
              BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2401748
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                                   20011004
                                                CA 2001-2401748
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     GB 2361236
                            A1
                                   20011017
                                                GB 2001-7758
                                                                          20010328
     GB 2361236
                            B2
                                   20020424
     EP 1274705
                            A1
                                   20030115
                                                EP 2001-915544
                                                                          20010328
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     HU 200300382
                                   20030628
                                                HU 2003-382
                            A2
                                                                          20010328
     JP 2003528872
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                                   20030930
                                                JP 2001-570655
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     NZ 521068
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                            Α
                                                NZ 2001-521068
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     US 2002019404
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                                                US 2001-823075
                                                                          20010329
     US 6531479
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                                   20030311
     US 2003149057
                            A1
                                   20030807
                                                US 2002-327540
                                                                          20021220
     US 6699854
                            B2
                                   20040302
PRAI GB 2000-7636
                            Α
                                   20000329
     GB 2000-15117
                                   20000620
                            Α
     WO 2001-GB1423
                                   20010328
     US 2001-823075
                            A3
                                   20010329
OS
     MARPAT 135:288789
     The invention relates to 2-substituted 4-heteroaryl-pyrimidines I and
AB
     their pharmaceutically acceptable salts [wherein: X1 = CH and X2 = S; or 1
     of X1 and X2 = S and the other = N; Z = NH, NHCO, NHSO2, NHCH2, CH2,
     CH2CH2, or CH:CH; R1, R2, R3 = H, alkyl, aryl, aralkyl, heterocyclyl,
     halo, NO2, cyano, OH, alkoxy, aryloxy, NH2, NHR', N(R')(R''), NHCOR', NH(aryl), N(aryl)2, COOH, COOR', COO(aryl), CONH2, CONHR', CON(R')(R''),
     CONH(aryl), CON(aryl)2, SO3H, SO2NH2, CF3, COR', or CO(aryl), wherein
     alkyl, aryl, aralkyl, heterocyclyl, and NH(aryl) groups may be further
     substituted with 1 or more halo, NO2, cyano, OH, OMe, NH2, COOH, CONH2,
     and/or CF3; at least 1 of R1 and R2 \neq H when either X1 or X2 = S;
     R4, R5, R6, R7, R8 = H, (un)substituted alkyl, halo, NO2, cyano, OH,
     (un) substituted alkoxy, NH2, NHR', alkyl-aryl, alkyl-heteroaryl,
     NH(C:NH)NH2, N(R')3+, N(R')(R''), COOH, COOR', CONH2, CONHR',
     CON(R')(R''), SO3H, SO2NH2, CF3, or (CH2)nO(CH2)mNR'R'',
     (CH2) nCO2 (CH2) mOR''' wherein n = 0, 1, 2, or 3; m = 1, 2 or 3; R', R'',
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R''' = alkyl]. The invention also relates to preparation of I, pharmaceutical compns. containing them, and their use as inhibitors of cyclin-dependant kinases (CDKs), and hence their use in the treatment of proliferative disorders such as cancer, leukemia, psoriasis and the like. Examples include 22 syntheses and a variety of bioassays. For instance, 4-FC6H4NH2 was treated with HNO3 and cyanamide in EtOH to give 47% 4-FC6H4NHC(:NH)NH2.HNO3 (II). Sep., 5-acetyl-2,4-dimethylthiazole was condensed with N,N-dimethylformamide di-Me acetal to give 79% 3-dimethylamino-1-(2,4-dimethylthiazol-5-yl)propenone (III). Cyclocondensation of II with III in refluxing MeOCH2CH2OH in the presence of NaOH gave title compound IV in 89% yield. In an assay against multiple kinases, IV selectively inhibited CDKs, showing an IC50 of 0.019  $\mu$ M against CDK2/cyclin E, and 0.47  $\mu$ M against CDK4/cyclin D1, vs. >20  $\mu$ M against PCK $\alpha$  and SAPK2a. Addnl. bioassays of I showed antiproliferative and cytotoxic activity.

IT 364334-28-1P 364334-31-6P 364334-32-7P 364334-35-0P 364334-36-1P 364334-37-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of heteroarylpyrimidines as CDK-inhibiting antiproliferative and anticancer agents)

RN 364334-28-1 CAPLUS

CN

2-Pyrimidinamine, 4-(2,4-dimethyl-5-thiazolyl)-N-(4-fluorophenyl)-6-phenyl-(9CI) (CA INDEX NAME)

RN 364334-31-6 CAPLUS

CN 2-Pyrimidinamine, 4-(2,4-dimethyl-5-thiazolyl)-N-(4-fluorophenyl)-6-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 364334-32-7 CAPLUS

CN 2-Pyrimidinamine, N-(4-chlorophenyl)-4-(2,4-dimethyl-5-thiazolyl)-6-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 364334-35-0 CAPLUS

CN 2-Pyrimidinamine, 4-(2,4-dimethyl-5-thiazolyl)-N-(4-fluorophenyl)-6-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 364334-36-1 CAPLUS

CN Phenol, 4-[6-(2,4-dimethyl-5-thiazolyl)-2-[(4-fluorophenyl)amino]-4-pyrimidinyl]-2,6-dimethoxy- (9CI) (CA INDEX NAME)

RN

364334-37-2 CAPLUS
Phenol, 4-[6-(2,4-dimethyl-5-thiazolyl)-2-[(4-fluorophenyl)amino]-4pyrimidinyl]- (9CI) (CA INDEX NAME) CN

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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T.4
     ANSWER 31 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2001:78219 CAPLUS
DN
     134:141718
     Pyrimidine derivative inhibitors of viral helicase
ΤI
     Hale, Michael; Maltais, Francois; Baker, Christopher; Janetka, James;
IN
     Moon, Young Choon; Saunders, Jeffrey
PA
     Vertex Pharmaceuticals Incorporated, USA
SO
     PCT Int. Appl., 43 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                            APPLICATION NO.
                                DATE
                                                                   DATE
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                                _____
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PΙ
     WO 2001007027
                          A2
                                20010201
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                                                                   20000719
     WO 2001007027
                         Α3
                                20010809
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             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI US 1999-145193P
                          Ρ
                                19990722
     US 1999-150783P
                          Ρ
                                19990826
     MARPAT 134:141718
OS
AΒ
     A method is provided which is useful for inhibiting viral helicases, in
     particular the hepatitis C virus NS3 helicase. The method employs compns.
     including I [X = S, NR5; n = 0, 1; T = bond, linker group; R1 = R, Ph,
     heterocyclyl; R2 = OR, halo, SR (when dotted line indicates double bond)
     or R2 = :0, :S (when dotted line indicates single bond); R3 = halo, CN,
     CO2H, CHO, etc.; R4 = 4-chlorophenyl, 2-thienyl, cyclohexyl, etc.; R5 = H,
     R, OR, etc.; R = H, C3-8 cycloalkyl, (un)branched C1-12 alkyl, etc.; when
     dotted line indicates single bond, attached ring N substituted by R5; any
     N may exist as N oxide; any heteroatom may be substituted with labile
     group for prodrug administration]. Preferred compds. are those where R3
     is an electron withdrawing group (e.g. halo, CN). More preferred are
     those compds. where R3 is an electron withdrawing group and R2 is OH.
     Most preferred are those compds. where R2 and R3 are as just described and
     X is S. In particular, the compns. and methods of this invention are
     useful in treating diseases caused by hepatitis C virus, bovine viral
     diarrhea virus or vaccinia virus.
IT
     273920-47-1
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
        (pyrimidine derivative inhibitors of viral helicase)
RN
     273920-47-1 CAPLUS
CN
     5-Pyrimidinecarbonitrile, 6-(4-chlorophenyl)-2-[(4-chlorophenyl)amino]-1,4-
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dihydro-4-oxo- (9CI) (CA INDEX NAME)

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L4
     ANSWER 32 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2000:911230 CAPLUS
     134:71598
DN
ΤI
     Preparation of 2-arylamino-5-cyanopyrimidines as inhibitors of KDR kinase
     and/or FGFr kinase.
     Batchelor, Mark James; Moffat, David Festus Charles; Davis, Jeremy Martin;
IN
     Hutchings, Martin Clive
PA
     Celltech Chiroscience Limited, UK
SO
     PCT Int. Appl., 102 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LΑ
FAN.CNT 1
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                                                                    DATE
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             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
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             YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
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     MARPAT 134:71598
os
     Title compds. [I; Ar = (substituted) aryl, heteroaryl; R1 = H, alkyl; R2 =
AB
     X1R3; X1 = bond, linker atom or group; R3 = (substituted) aliphatic,
     cycloaliph., heteroaliph., heterocycloaliph., aromatic or heteroarom. group]
     and the salts, solvates, hydrates and N-oxides thereof, were prepared Thus,
     3,4,5-trimethoxyphenylguanidinium nitrate (preparation given),
     1-phenyl-2-cyano-3-dimethylaminopropen-1-one, and NaOH were refluxed in
```

EtOH to give 5-cyano-4-phenyl-N-(3,4,5-trimethoxyphenyl)pyrimidin-2-amine.

I inhibited KDR kinase and FGFr kinase with IC50  $\leq$ 1  $\mu$ M.

314267-54-4P 314267-59-9P 314267-61-3P

IT

CN

RN 314267-59-9 CAPLUS

5-Pyrimidinecarbonitrile, 2-[(4-fluorophenyl)amino]-4-[4-[1-methyl-1-(1-pyrrolidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 314267-61-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[4-(1-amino-1-methylethyl)phenyl]-2-[(3-fluorophenyl)amino]- (9CI) (CA INDEX NAME)

RN 314268-67-2 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[4-(1-amino-1-methylethyl)phenyl]-2-[(3,5-difluorophenyl)amino]- (9CI) (CA INDEX NAME)

RN 314268-68-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[4-(1-amino-1-methylethyl)phenyl]-2-[(3-fluoro-4-methylphenyl)amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} NH2 & F \\ Me & NH \\ \hline \\ Me & NH \\ \hline \end{array}$$

RN 314268-69-4 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[4-(1-amino-1-methylethyl)phenyl]-2-[(3,4,5-trifluorophenyl)amino]- (9CI) (CA INDEX NAME)

RN 314268-70-7 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[4-(1-amino-1-methylethyl)phenyl]-2-[[4-fluoro-3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)

RN 314268-71-8 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[4-(1-amino-1-methylethyl)phenyl]-2-[(2,4-difluorophenyl)amino]- (9CI) (CA INDEX NAME)

RN 314268-72-9 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[4-(1-amino-1-methylethyl)phenyl]-2-[(3,4-difluorophenyl)amino]- (9CI) (CA INDEX NAME)

RN 314268-73-0 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[4-(1-amino-1-methylethyl)phenyl]-2-[(3-chloro-4-fluorophenyl)amino]- (9CI) (CA INDEX NAME)

RN 314268-74-1 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[4-(1-amino-1-methylethyl)phenyl]-2-[[3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)

RN 314269-19-7 CAPLUS

CN Acetamide, N-[1-[4-[5-cyano-2-[(4-fluorophenyl)amino]-4-pyrimidinyl]phenyl]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 314269-20-0 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[4-[1-(dimethylamino)-1-methylethyl]phenyl]-2-[(4-fluorophenyl)amino]- (9CI) (CA INDEX NAME)

RN 314269-21-1 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-[(3-fluorophenyl)amino]-4-[4-(1H-imidazol-1-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 314269-23-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-[(3-chloro-4-methylphenyl)amino]-4-phenyl-(9CI) (CA INDEX NAME)

RN 314269-25-5 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-[[4-chloro-3-(trifluoromethyl)phenyl]amino]-4-phenyl- (9CI) (CA INDEX NAME)

IT 314267-93-1P 314267-94-2P 314267-95-3P

314267-96-4P 314267-97-5P 314267-98-6P

314267-99-7P 314268-00-3P 314268-01-4P

314268-02-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2-arylamino-5-cyanopyrimidines as inhibitors of KDR kinase and/or FGFr kinase)

RN 314267-93-1 CAPLUS

CN Carbamic acid, [1-[4-[5-cyano-2-[(3,5-difluorophenyl)amino]-4-pyrimidinyl]phenyl]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CAINDEX NAME)

RN 314267-94-2 CAPLUS

CN Carbamic acid, [1-[4-[5-cyano-2-[(3-fluoro-4-methylphenyl)amino]-4-pyrimidinyl]phenyl]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 314267-95-3 CAPLUS

CN Carbamic acid, [1-[4-[5-cyano-2-[(3,4,5-trifluorophenyl)amino]-4-pyrimidinyl]phenyl]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 314267-96-4 CAPLUS

CN Carbamic acid, [1-[4-[5-cyano-2-[[4-fluoro-3-(trifluoromethyl)phenyl]amino ]-4-pyrimidinyl]phenyl]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 314267-97-5 CAPLUS

CN Carbamic acid, [1-[4-[5-cyano-2-[(2,4-difluorophenyl)amino]-4pyrimidinyl]phenyl]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 314267-98-6 CAPLUS

CN Carbamic acid, [1-[4-[5-cyano-2-[(3,4-difluorophenyl)amino]-4-pyrimidinyl]phenyl]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 314267-99-7 CAPLUS

CN Carbamic acid, [1-[4-[2-[(3-chloro-4-fluorophenyl)amino]-5-cyano-4-pyrimidinyl]phenyl]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 314268-00-3 CAPLUS

CN Carbamic acid, [1-[4-[5-cyano-2-[(4-fluorophenyl)amino]-4-pyrimidinyl]phenyl]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 314268-01-4 CAPLUS

CN Carbamic acid, [1-[4-[5-cyano-2-[[3-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]phenyl]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 314268-02-5 CAPLUS

CN Carbamic acid, [1-[4-[5-cyano-2-[(3-fluorophenyl)amino]-4-pyrimidinyl]phenyl]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CAINDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

L4 ANSWER 33 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:835377 CAPLUS

DN 134:17494

TI Preparation of aryl-substituted pyrimidines as insecticidal and acaricidal agents

IN Wood, William Wakefield; Fleming, Linda; Cuccia, Salvatore John

PA American Cyanamid Company, USA

SO U.S., 10 pp., Division of U.S. Ser. No. 36,490. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

T. LTIA	CNI Z				
PATENT NO.		KIND	DATE	APPLICATION NO.	DATE
PI	US 6153619	Α	20001128	US 1999-273942	19990322
	US 6306866	B1	20011023	US 1998-36490	19980306
PRAI	US 1998-36490	<b>A</b> 3	19980306		

OS MARPAT 134:17494

AB The title compds. [I; R1 = H, halo, alkyl, etc.; A = substituted Ph; B = substituted Ph; with the proviso that either A or B must be substituted by at least one halogen atom; one of Y and Z = N and the other = CR2; R2 = R1; X = O, NR; R = H, alkyl], useful for the control of insect and acarid pests (biol. data given), were prepared E.g., a 2-step synthesis of I [Y = N; Z = CH; R1 = H; X = O; A = 3-F3CC6H4; B = 3,4-Cl2C6H3] was presented.

IT 309255-89-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of aryl-substituted pyrimidines as insecticidal and acaricidal agents)

RN 309255-89-8 CAPLUS

CN 2-Pyrimidinamine, N,4-bis[4-fluoro-3-(trifluoromethyl)phenyl]-N-methyl-(9CI) (CA INDEX NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

## 10/501,445

L4ANSWER 34 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN2000:585430 CAPLUS

DN 133:150583

Preparation of phenylpyrimidine and phenyltriazine derivatives as ΤI fungicides

IN. Kumita, Izumi; Noda, Kaoru

PΑ Nippon Soda Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 10 pp. CODEN: JKXXAF

DΤ Patent

LA Japanese

FAN.CNT 1							
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE /		
					- <b>-</b>		
PI	JP 2000229949	. A2	20000822	JP 1999-33002	19990210		
PRAI	JP 1999-33002		19990210		<i></i>		

MARPAT 133:150583 OS

Title compds. I (R1, R2 = H, halo; R3 = Ph, pyridyl, cycloalkyl, etc.; R4 AB = H, cyano, halo, alkyl, alkoxy, alkoxycarbonyl, alkylthio, alkylsulfinyl, alkylsulfonyl, amino), useful as fungicides, are prepared Thus, reaction of 1,1-bis(methylthio)-3-(2,6-dichlorophenyl)propen-3-one with 4-chlorophenylguanidine nitrate in DMF in the presence of K2CO3 gave 4-(2,6-dichlorophenyl)-2-(4-chlorophenylamino)-6-methylthiopyrimidine, reaction of which with NaBH4 in EtOH in the presence of NiCl2 and aqueous NaOH gave 4-(2,6-dichlorophenyl)-2-(4-chlorophenylamino)pyrimidine (II). II showed fungicidal activity against Botrytis cinerea.

ΙT 287720-02-9P 287720-04-1P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of phenylpyrimidine and phenyltriazine derivs. as fungicides)

RN 287720-02-9 CAPLUS

CN 2-Pyrimidinamine, N-(4-chlorophenyl)-4-(2,6-dichlorophenyl)-6-(methylthio)-(CA INDEX NAME)

RN287720-04-1 CAPLUS

CN 2-Pyrimidinamine, N-(4-chlorophenyl)-4-(2,6-dichlorophenyl)-6-(methylsulfonyl) - (9CI) (CA INDEX NAME)

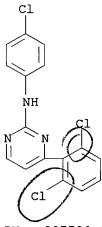
IT 287720-03-0P 287720-05-2P 287720-06-3P

287720-08-5P 287720-09-6P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of phenylpyrimidine and phenyltriazine derivs. as fungicides)

RN 287720-03-0 CAPLUS

CN 2-Pyrimidinamine, N-(4-chlorophenyl)-4-(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



RN 287720-05-2 CAPLUS

CN 2-Pyrimidinamine, N-(4-chlorophenyl)-4-(2,6-dichlorophenyl)-6-methoxy-(9CI) (CA INDEX NAME)

RN 287720-06-3 CAPLUS

CN 4-Pyrimidinecarbonitrile, 2-[(4-chlorophenyl)amino]-6-(2,6-dichlorophenyl)-(9CI) (CA INDEX NAME)

RN 287720-08-5 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 2-[(4-chlorophenyl)amino]-6-(2,6-dichlorophenyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 287720-09-6 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-6-(2,6-dichlorophenyl)-N4,N4-dimethyl- (9CI) (CA INDEX NAME)

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T.4
     ANSWER 35 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2000:513679 CAPLUS
DN
     133:120681
     Preparation of amino acid acyl derivatives as inhibitors of leukocyte
ΤI
     adhesion mediated by VLA-4
     Konradi, Andrei; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan;
     Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen,
     Darren B.; Grant, Francine S.; Semko, Christopher; Xu, Ying-Zi
PA
     Elan Pharmaceuticals, Inc., USA; American Home Products
SO
     PCT Int. Appl., 342 pp.
     CODEN: PIXXD2
DΤ
     Patent
     English
LΑ
FAN.CNT 2
     PATENT NO.
                          KIND
                                 DATE
                                             APPLICATION NO.
                                                                     DATE
     ______
                          ____
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PΙ
     WO 2000043372
                           A1
                                 20000727
                                             WO 2000-US1686
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         W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
             SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
              DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
              CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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     EP 1144388
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              IE, SI, LT, LV, FI, RO
     BR 2000007663
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                                 20021112
                                             US 2000-489378
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     US 6492372
                           В1
                                 20021210
                                             US 2000-489377
                                                                     20000121
     HU 200201213
                           A2
                                 20021228
                                             HU 2002-1213
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     AU 773538
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                                 20040527
                                             AU 2000-34724
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     TW 239954
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                                 20050921
                                             TW 2000-89101088
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     ZA 2001005314
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                                 20030327
                                             ZA 2001-5314
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     NO 2001003600
                           Α
                                 20010920
                                             NO 2001-3600
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     US 2003125324
                           A1
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                                             US 2002-218366
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     US 6911439
                           B2
                                 20050628
     US 2003144328
                           A1
                                 20030731
                                             US 2002-218445
                                                                     20020815
     US 6903088
                           B2
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     US 2003139402
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                                             US 2002-251442
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     US 7049306
                           B2
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     HK 1046132
                           Α1
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     NZ 529822
                           Α
                               20031219
                                             NZ 2003-529822
                                                                     20031127
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                                                                     20031229
     US 7005433
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     US 2005203093
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                                 20050915
                                             US 2005-33079
                                                                     20050110
     US 2005261293
                           Α1
                                 20051124
                                             US 2005-145489
                                                                     20050602
PRAI US 1999-116923P
                           A2
                                 19990122
     US 1999-160999P
                           Ρ
                                 19991021
                           Ρ
     US 1999-160199P
                                 19991019
     US 2000-489377
                           A3
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     US 2000-489378
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     WO 2000-US1686
                           W
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     US 2002-218366
                           A3
                                 20020815
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20020815

20020920

US 2002-218445

US 2002-251442

A3

**A**1

OS MARPAT 133:120681

AB Disclosed are compds. R2-W:CR1-Q-CR3R3'COX and R2-W'-CHR1-Q-CR3R3'COX [R1 and R2 are joined to form a ring; R3, R3' = H, iso-Pr, -CH2Z or :CHZ, where Z = H, acylamino, alkyl, alkoxy, aryloxy, aryl, aryloxyaryl, carboxy, carboxyalkyl, etc.; Q = O, S, SO, SO2, NH or imino group; W = nitrogen, carbon; W' = nitrogen, carbon, oxygen, sulfur, SO, SO2; X = OH, (un)substituted alkoxy, alkenoxy, cycloalkoxy, cycloalkenoxy, aryloxy, heteroaryloxy or heterocyclyloxy, an amino group] which bind VLA-4. Thus, N-[5-(N-4-toluenesulfonylamino)pyrimidin-4-yl]-L-4-(N,N-dimethylcarbamyloxy)phenylalanine tert-Bu ester was prepared by condensation of L-4-(N,N-dimethylcarbamyloxy)phenylalanine tert-Bu ester with 2,4-dichloro-5-nitropyrimidine, followed by nitro group reduction and tosylation. Compds. synthesized in the examples are expected to have a binding affinity to VLA-4 expressed by an IC50 of 15 μM or less.

IT 285139-65-3P 285140-62-7P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amino acid acyl derivs. as inhibitors of leukocyte adhesion mediated by VLA-4)

RN 285139-65-3 CAPLUS

CN L-Tyrosine, N-[2-[(4-chlorophenyl)methylamino]-5-(2-methylphenyl)-4-pyrimidinyl]-, dimethylcarbamate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 285140-62-7 CAPLUS

CN [1,1'-Biphenyl]-4-propanoic acid,  $\alpha$ -[[2-[(4-chlorophenyl)methylamino]-5-(2,4,6-trimethylphenyl)-4-pyrimidinyl]amino]-2',6'-dimethoxy-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L4
     ANSWER 36 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
ΑN
     1999:495258 CAPLUS
DN
     131:129907
ΤI
     Preparation and formulation of tricyclic compounds as immunosuppressants
     and allergy inhibitors
IN
     Tanimoto, Norihiko; Hasegawa, Yasushi; Haga, Nobuhiro
PA
     Shionogi & Co., Ltd., Japan
     PCT Int. Appl., 298 pp.
SO
     CODEN: PIXXD2
DΤ
     Patent
LA
     Japanese
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
                                            _____
PΙ
     WO 9938829
                         A1
                                19990805
                                            WO 1999-JP297
                                                                   19990126
        W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
             KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW,
            MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR,
             TT, UA, UG, US, UZ, VN, YU, ZW
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
             CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2318368
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             IE, SI, LT, LV, FI, RO
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                          Α
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     TR 200002225
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     HU 200103304
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                                            NZ 1999-506101
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                                            RU 2000-121556
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                                            NO 2000-3706
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                                            US 2000-600790
                          В1
                                                                   20000721
PRAI JP 1998-15554
                          Α
                                19980128
     WO 1999-JP297
                          W
                                19990126
OS
     MARPAT 131:129907
AB
     The title compds. I [each of ring A, ring B and ring C is independently a
     substituted or unsubstituted aromatic ring or a substituted or unsubstituted
     five or six-membered heterocycle which may be condensed with a benzene
     ring; when ring A, ring B and/or ring C is a substituted or unsubstituted
     five-membered heterocycle, W1, W2 and/or W3 represents a bond; X is O or
     NR1 (where R1 is hydrogen, a lower alkyl or the like); Y is hydrogen, a
     lower alkyl, a lower alkenyl or the like; one of V1 and V2 is a single
     bond and the other is a single bond, O, etc.] are prepared The title compound
     II in vitro showed IC50 of 400 ng/mL against the growth of mouse EL4
     cells. The inhibiting activities of compds. of this invention against the
     production of IgE were also demonstrated.
IT
     234429-03-9P 234429-04-0P 234429-05-1P
     234429-06-2P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of tricyclic compds. as immunosuppressants and allergy
        inhibitors)
```

RN

234429-03-9 CAPLUS

CN Phenol, 5-[2-[(4-fluorophenyl)amino]-4-methoxy-6-methyl-5-pyrimidinyl]-2-[(4-methylphenyl)methoxy]- (9CI) (CA INDEX NAME)

RN 234429-04-0 CAPLUS

CN Phenol, 5-[2-[(4-fluorophenyl)amino]-4-methoxy-6-methyl-5-pyrimidinyl]-2[(4-methylphenyl)methoxy]-, methanesulfonate (ester) (9CI) (CA INDEX NAME)

RN 234429-05-1 CAPLUS

CN Phenol, 5-[2-[(4-fluorophenyl)amino]-4-methoxy-6-methyl-5-pyrimidinyl]-2-[(3-methyl-2-butenyl)oxy]- (9CI) (CA INDEX NAME)

$$Me_2C = CH - CH_2 - O$$
 $Me$ 
 $N$ 
 $N$ 
 $N$ 
 $N$ 

RN 234429-06-2 CAPLUS

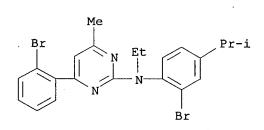
CN Phenol, 5-[2-[(4-fluorophenyl)amino]-4-methoxy-6-methyl-5-pyrimidinyl]-2[(3-methyl-2-butenyl)oxy]-, methanesulfonate (ester) (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me-S-O} \\ \text{Me-S-O} \\ \text{Me} \\ \text{O} \\ \text{N} \end{array}$$

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- T.4 ANSWER 37 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
- ΑN 1999:295954 CAPLUS
- DN 131:5238
- TΙ 4-Aryl-2-anilinopyrimidines as corticotropin-releasing hormone (CRH) antagonists
- ΑU Cocuzza, Anthony J.; Hobbs, Frank W.; Arnold, Charles R.; Chidester, Dennis R.; Yarem, Jerry A.; Culp, Steven; Fitzgerald, Lawrence; Gilligan, Paul J.
- CS Chemical and Physical Sciences Department, DuPont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA
- SO Bioorganic & Medicinal Chemistry Letters (1999), 9(7), 1057-1062 CODEN: BMCLE8; ISSN: 0960-894X
- Elsevier Science Ltd. PB
- DTJournal
- LA English
- AΒ A series of 4-aryl-2-(N-ethylanilino)pyrimidines has been synthesized as corticotropin-releasing hormone inhibitors. The effect of substitution on each aromatic ring on receptor binding was investigated.
- 219840-42-3P 219840-43-4P 219840-45-6P IT
  - 219840-46-7P 219840-47-8P 219840-48-9P
  - 219840-49-0P 219840-50-3P 219840-51-4P
  - 219840-52-5P 219840-53-6P 219840-54-7P
  - 219840-55-8P 219840-56-9P 219840-57-0P
  - 219840-59-2P 219840-60-5P 219840-61-6P
  - 219840-62-7P 219840-63-8P 219840-64-9P 219840-65-0P 219840-82-1P 219840-83-2P

  - 225922-77-0P 225922-78-1P 225922-79-2P 225922-80-5P 225922-83-8P 225922-84-9P
  - RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
    - (2-anilino-4-arylpyrimidines as corticotropin-releasing hormone antagonists)
- RN 219840-42-3 CAPLUS
- 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-4-(2-bromophenyl)-N-CN ethyl-6-methyl- (9CI) (CA INDEX NAME)





- RN 219840-43-4 CAPLUS
- 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-4-(2-chlorophenyl)-N-CN ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-45-6 CAPLUS

CN 2-Pyrimidinamine, N-(2-bromo-4,6-dimethoxyphenyl)-N-ethyl-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-46-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-47-8 CAPLUS

CN 1,4-Benzenediamine, 2-bromo-N1-ethyl-6-methoxy-N4,N4-dimethyl-N1-[4-methyl-6-[2-(trifluoromethyl)phenyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 219840-48-9 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-

## [3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

$$r_{3}$$
C  $r_{3}$ C  $r_{3}$ C  $r_{4}$ C  $r_{4}$ C  $r_{5}$ C  $r$ 

RN 219840-49-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-50-3 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-(2-fluorophenyl)-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-51-4 CAPLUS

CN 2-Pyrimidinamine, N-(2-bromo-4,6-dimethoxyphenyl)-4-(2-chlorophenyl)-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-52-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-(2-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 219840-53-6 CAPLUS

CN 2-Pyrimidinamine, 4-(2-aminophenyl)-N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-54-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-[2-(methylamino)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-55-8 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-4-[2-(dimethylamino)phenyl]-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-56-9 CAPLUS

CN 2-Pyrimidinamine, N-(2,4-dibromophenyl)-N-ethyl-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-57-0 CAPLUS

CN Ethanone, 1-[3-bromo-4-[ethyl[4-methyl-6-[2-(trifluoromethyl)phenyl]-2-pyrimidinyl]amino]phenyl]- (9CI) (CA INDEX NAME)

RN 219840-59-2 CAPLUS

CN Benzonitrile, 2-[2-[[2-bromo-4-(1-methylethyl)phenyl]ethylamino]-6-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 219840-60-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-

[2-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-61-6 CAPLUS

CN Benzoic acid, 2-[2-[[2-bromo-4-(1-methylethyl)phenyl]ethylamino]-6-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 219840-62-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(methylthio)phenyl]-N-ethyl-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-63-8 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(methylsulfonyl)phenyl]-N-ethyl-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-64-9 CAPLUS

CN 2-Pyrimidinamine, N-(2-bromo-4,6-dimethoxyphenyl)-N-ethyl-4-(2-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-65-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

RN 219840-82-1 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-(2-methylphenyl)- (9CI) (CA INDEX NAME)

RN 219840-83-2 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-4-(2,6-

dichlorophenyl)-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 225922-77-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-phenyl- (9CI) (CA INDEX NAME)

RN 225922-78-1 CAPLUS

CN 2-Pyrimidinamine, 4-[1,1'-biphenyl]-2-yl-N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 225922-79-2 CAPLUS

CN 2-Pyrimidinamine, 4-[1,1'-biphenyl]-3-yl-N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 225922-80-5 CAPLUS

CN 2-Pyrimidinamine, 4-[1,1'-biphenyl]-4-yl-N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 225922-83-8 CAPLUS

CN Benzenaminium, 2-[2-[[2-bromo-4-(1-methylethyl)phenyl]ethylamino]-6-methyl-4-pyrimidinyl]-N,N,N-trimethyl-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 225922-82-7 CMF C25 H32 Br N4

CM 2

CRN 37181-39-8 CMF C F3 O3 S

RN 225922-84-9 CAPLUS

CN 2-Pyrimidinamine, N-(2-bromo-4,6-dimethoxyphenyl)-N-ethyl-4-methyl-6-phenyl- (9CI) (CA INDEX NAME)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 38 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
     1999:48709 CAPLUS
AN
DN
     130:125084
ΤI
     Aryl- and arylamino-substituted heterocycles as corticotropin releasing
     hormone (CRF) antagonists
IN
     Cocuzza, Anthony J.; Hobbs, Frank W.; Beck, James P.; Gilligan, Paul J.
PΑ
     Du Pont Pharmaceuticals Company, USA
SO
     PCT Int. Appl., 86 pp.
     CODEN: PIXXD2
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                                19980702
OS
     MARPAT 130:125084
AΒ
     Corticotropin releasing factor (CRF) antagonists I and their stereoisomers
     and pharmaceutically acceptable salts are disclosed [wherein Y = CR2 or N;
     Z = CH \text{ or } N; K = CR5 \text{ or } N; R1 = alk(en/yn)yl, Cl, F, cyano, CF3; R2R4 =
     E-F where E and F = CR9 and/or CR9'; or R2R4 = A:D where A and D = CH,
     CR10, or N, provided that A:D is oriented to form imidazole but not
     pyrazole; or R2R4 = A-D where A = NR9 and D = CO, oriented to form an
     imidazolone; R3 = Ph, naphthyl, pyridinyl, or pyrimidinyl, all substituted
     by R8; R4 = (un)substituted alkyl, allyl, or propargyl; R5 = 1-4 of
     alk(en/yn)yl, cycloalkyl, halo, NO2, cyano, NR6R7, OR7, COR7, C(:NOR9)R7,
     SOnR7, etc.; or 2 R5 moieties may form CR9R9'CR9R9'O, CR9:CR9'O, etc.; R6,
     R7 = H or (un) substituted alkyl, cycloalkyl, (CH2) mPh or
     (CH2)m-heteroaryl; R8 = alk(en/yn)yl, cycloalkyl, Ph, heteroaryl, halo,
     NO2, cyano, NR6R7, OR7, etc., with provisos; R9, R9' = H, alkyl; n = 0-2;
     m = 0-6]. Also disclosed is their use in treating psychiatric disorders
     and neurol. diseases, anxiety-related disorders, post-traumatic stress
     disorder, supranuclear palsy and feeding disorders, as well as treatment
     of immunol., cardiovascular or heart-related diseases, and colonic
     hypersensitivity associated with psychopathol. disturbance and stress in
     mammals. For example, condensation of 2-BrC6H4COCH3 with MeC(OMe)2NMe2
     gave 2-BrC6H4COCH: MeNMe2, which underwent cyclocondensation with
     (2-bromo-4-isopropylphenyl) quanidine-HCl, followed by N-alkylation of the
     resultant aminopyrimidine with EtI and NaH in DMSO, to give title compound
     II. Some I were active (no data) in an assay for inhibition of
     CRF-stimulated adenylate cyclase activity.
     219840-85-4P 219840-87-6P 219840-90-1P
IT
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(Reactant or reagent)
(intermediate; preparation of aryl-and arylamino-substituted heterocycles as

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

219840-92-3P

corticotropin releasing hormone antagonists)

RN 219840-85-4 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-4-(2-bromophenyl)-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-87-6 CAPLUS

CN 2-Pyrimidinamine, N-(2-bromo-4,6-dimethoxyphenyl)-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-90-1 CAPLUS

CN 2-Pyrimidinamine, N-(2-bromo-4,6-dimethoxyphenyl)-4-(2-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-92-3 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-4-methyl-6-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

RN 219840-43-4 CAPLUS
CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-4-(2-chlorophenyl)-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-44-5 CAPLUS

CN 1,4-Benzenediamine, 2-bromo-N1-[4-(2-chlorophenyl)-6-methyl-2-pyrimidinyl]-N1-ethyl-6-methoxy-N4,N4-dimethyl- (9CI) (CA INDEX NAME)

RN 219840-45-6 CAPLUS

CN 2-Pyrimidinamine, N-(2-bromo-4,6-dimethoxyphenyl)-N-ethyl-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-46-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-47-8 CAPLUS

CN 1,4-Benzenediamine, 2-bromo-N1-ethyl-6-methoxy-N4,N4-dimethyl-N1-[4-methyl-

6-[2-(trifluoromethyl)phenyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 219840-48-9 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-49-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-50-3 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-(2-fluorophenyl)-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-51-4 CAPLUS

CN 2-Pyrimidinamine, N-(2-bromo-4,6-dimethoxyphenyl)-4-(2-chlorophenyl)-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-52-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-(2-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 219840-53-6 CAPLUS

CN 2-Pyrimidinamine, 4-(2-aminophenyl)-N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-54-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-[2-(methylamino)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-55-8 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-4-[2-(dimethylamino)phenyl]-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-56-9 CAPLUS

CN 2-Pyrimidinamine, N-(2,4-dibromophenyl)-N-ethyl-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-57-0 CAPLUS

CN Ethanone, 1-[3-bromo-4-[ethyl[4-methyl-6-[2-(trifluoromethyl)phenyl]-2-pyrimidinyl]amino]phenyl]- (9CI) (CA INDEX NAME)

RN 219840-59-2 CAPLUS

CN Benzonitrile, 2-[2-[[2-bromo-4-(1-methylethyl)phenyl]ethylamino]-6-methyl-

4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 219840-60-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-[2-(1H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-61-6 CAPLUS

CN Benzoic acid, 2-[2-[[2-bromo-4-(1-methylethyl)phenyl]ethylamino]-6-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 219840-62-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(methylthio)phenyl]-N-ethyl-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-63-8 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(methylsulfonyl)phenyl]-N-ethyl-4-methyl-6-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-64-9 CAPLUS

CN 2-Pyrimidinamine, N-(2-bromo-4,6-dimethoxyphenyl)-N-ethyl-4-(2-methoxyphenyl)-6-methyl- (9CI) (CA INDEX NAME)

RN 219840-65-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

RN 219840-66-1 CAPLUS

CN 2-Pyrimidinamine, N-(2,4-dibromophenyl)-N-ethyl-4-methyl-6-[2-

(methylthio)phenyl] - (9CI) (CA INDEX NAME)

RN 219840-67-2 CAPLUS

CN 2-Pyrimidinamine, N-(2,4-dibromophenyl)-N-ethyl-4-methyl-6-[2-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

RN 219840-82-1 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-N-ethyl-4-methyl-6-(2-methylphenyl)- (9CI) (CA INDEX NAME)

RN 219840-83-2 CAPLUS

CN 2-Pyrimidinamine, N-[2-bromo-4-(1-methylethyl)phenyl]-4-(2,6-dichlorophenyl)-N-ethyl-6-methyl- (9CI) (CA INDEX NAME)

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ANSWER 39 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
AN
    1998:394334 CAPLUS
DΝ
     129:67791
     Preparation of 2-substituted 5-(4-fluorophenyl)-4-(4-pyridyl)pyrimidines
ΤI
     and related compounds as drugs
IN
     Spohr, Ulrike D.; Malone, Michael J.; Mantlo, Nathan B.
    Amgen Inc., USA; Spohr, Ulrike D.; Malone, Michael J.; Mantlo, Nathan B.
PA
SO
     PCT Int. Appl., 232 pp.
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OS MARPAT 129:67791

Novel pyrimidines [I; R1, R2 = ZY, with a proviso; Z = bond, AB (un) substituted alk(en)yl, alkynyl, (un) substituted heterocyclyl, (un) substituted (hetero) aryl; etc; Y = H, halo, NO2, COR20, CNR5NR5R21, OR21, O2CR21, etc.; R5 = H, (un)substituted alk(en)yl, alkynyl, cycloalkyl, (hetero)aryl, etc.; R20 = (un)substituted alk(en)yl, alkynyl, aralkoxy, aralkylthio, aralkylsulfonyl, etc.; R21 = H, any of definitions for R20] and their pharmaceutically acceptable salts, effective for prophylaxis and treatment of diseases mediated by tumor necrosis factor  $\alpha$  (TNF- $\alpha$ ), IL-1 $\beta$ , IL-6 and/or IL-8 and other maladies, e.g., pain and diabetes, were prepared, e.g., by enamination of 2-(4-fluorophenyl)-1-(4-pyridinyl)ethanone (II) with (Me2N)2CHOMe and cyclocondensation of the resulting (dimethylamino)propenone with an amidine, guanidine or urea. I analogs, prodrugs, pharmaceutical compns., methods for prophylaxis and treatment of diseases or conditions involving inflammation, pain, diabetes, etc., and processes for making such compds. and their intermediates are also claimed. For example, heating a mixture of II with (Me2N) 2CHOMe at  $110^{\circ}$  for 1.5 h under Ar gave 3-(dimethylamino)-2-(4-fluorophenyl)-1-(4-pyridyl)-3-propen-1-one which was cyclocondensed with 4-pyridylamidine (prepared in situ from pyridylamidine-HCl and Na) by refluxing in EtOH to give a title compound I (R1 = R12 = 4-pyridinyl, R2 = H, R11 = 4-FC6H4). The latter in mice inhibited lipopolysaccharide-induced  $TNF-\alpha$  release with IC50 ≤20 μM.

IT 208935-17-5P 208935-23-3P 208935-27-7P

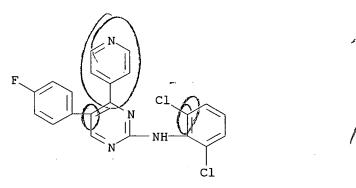
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-substituted (fluorophenyl) (pyridyl) pyrimidines and related compds. as drugs)

RN 208935-17-5 CAPLUS

CN

2-Pyrimidinamine, N-(2,6-dichlorophenyl)-5-(4-fluorophenyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



RN 208935-23-3 CAPLUS

CN 2-Pyrimidinamine, N,5-bis(4-fluorophenyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 208935-27-7 CAPLUS

CN 2-Pyrimidinamine, 5-(4-fluorophenyl)-4-(4-pyridinyl)-N-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

## 10/501,445

L4 ANSWER 40 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1996:465572 CAPLUS

DN 125:221772

TI Fused cyanopyrimidines. Part II. Synthesis and reactions of fused cyanopyrimidine derivatives as affecting enzymic agents

AU Abdel-Aziz, S. A.; Allimony, H. A.; El-Shaaer, H. M.; Ali, Usama F.; Abdel-Rahman, R. M.

CS Fac. Educ., Ain-Shams Univ., Cairo, Egypt

SO Phosphorus, Sulfur and Silicon and the Related Elements (1996), 113(1-4), 67-77

CODEN: PSSLEC; ISSN: 1042-6507

PB Gordon & Breach

DT Journal

LA English

Some new fused heterobicyclic systems, such as thiazolo[3,2-a]-pyrimidin-AB one (I; R = Ph, X = S, X1 = CH), 2,3-tetrahydrothiazolo[3,2-a]pyri/midin-5one (II; X2 = S), 2,4-tetrahydrothiazino[3,2-a]pyrimidin-3,6-dione (III; Y = Y2 = H,H, Y1 = O), 3-hydrothiazino[3,2-a]pyrimidin-2,4,6-trione (III; Y = Y2 = O, Y1 = H,H), 3-arylidenethiazino[3,2-a]pyrimidin-2,4,6/trione (III; Y = Y2 = 0, Y1 = CHC6H4Cl-4) and/or the related nitrogen compds. such as 2,3-tetrahydroimidazolo[3,2-a]pyrimidin-5-one (II; X2 = NH), 1-aryl-2,3-tetrahydroimidazolo[3,2-a]pyriminin-5-one (II; X2 = NC6H4Cl-4), quinazolino[3,2-a]pyrimidin-6,8-dione (IV) and 3-mercapto-1,2,4triazolo[4,3-a]pyrimidin-5-one (I; R = SH, X = NH, X1 = N) have been synthesized by the interaction of 2-mercapto-4-arylidene-5-cyanopyrimidin-6(1H) one (V) with  $\alpha,\beta$ -bifunctional nitrogen, oxygen and/or sulfur compds. The structures have been characterized by elemental analyses, IR, UV, 1H NMR and mass spectra data. Some newly prepared compds. revealed a moderate effect on the activity of cellobiase produced by Aspergillus nidulans.

IT 181175-85-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (synthesis and reactions of fused cyanopyrimidine derivs. as affecting enzymic agent)

RN 181175-85-9 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-[(4-chlorophenyl)amino]-6-(2,4-dichlorophenyl)-1,4-dihydro-4-oxo-(9CI) (CA INDEX NAME)

- L4 ANSWER 41 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1990:478409 CAPLUS
- DN 113:78409
- TI (Morpholinocarbonyl)benzothiophenes and analogs as agrochemical fungicides and their preparation
- IN Pepin, Regis; Schmitz, Christian; Lacroix, Guy Bernard; Dellis, Philippe; Veyrat, Christine
- PA Rhone-Poulenc Agrochimie, Fr.
- SO Eur. Pat. Appl., 75 pp. CODEN: EPXXDW
- DT Patent
- LA French
- FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 360701	A1	19900328	EP 1989-420320	19890831
	R: AT, BE, CH,	DE, ES	, FR, GB,	GR, IT, LI, LU, NL, SE	. /
	FR 2635776	A1	19900302	FR 1988-11665	19880901
	FR 2635776	B1	19930611		•
	FR 2648459	A1	19901221	FR 1989-5774	19890425
	FR 2648459	B1	19940527		
	FR 2649107	A1	19910104	FR 1989-9150	19890703
	FR 2649107	B1	19940819		
	FR 2649699	A1	19910118	FR 1989-9742	19890713
	HU 207931	В	19930728	HU 1989-4523	19890831
PRAI	FR 1988-11665	A	19880901		,
	FR 1989-5774	Α	19890425		
	FR 1989-9150	Α	19890703		
	FR 1989-9742	A	19890713		
OS	CASPEACT 113.78409.	Μάρραπ	113.79/00		

OS CASREACT 113:78409; MARPAT 113:78409

AB The title compds. I [ring A is a (substituted) C or heterocyclic ring containing ≥1 unsatd. bond, such as ethylene or aromatic; Y = O, S; Z = NR1R2; R1, R2 = (substituted) alkyl, alkoxy, C3-7 cycloalkyl, alkenyl, C3-7 alkynyl; or NR1R2 = (un)saturated (substituted) heterocyclyl; R3-R5 = H, halo, (substituted) amino, (substituted) alkyl, alkoxy, etc.; R3 and R4 (in meta and para positions) together may form a single radical containing 1 or 2 O atoms] were prepared A mixture of benzothiophene II (R = NH2) and NaNO2 in H2O containing H2SO4 was stirred for 1 h and then mixed with aqueous

KI. The resulting mixture was heated at 60° for 1 h to give II (R = iodo). At 1000 ppm, 69 compds. I [e.g. II (R = NO2)] gave 80% inhibition of Phythophthora infestans.

IT 128568-04-7P 128568-05-8P 128568-06-9P 128568-07-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as agrochem. fungicide)

RN 128568-04-7 CAPLUS

CN Morpholine, 4-[[2-[(4-chlorophenyl)amino]-4-(3,4-dimethoxyphenyl)-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 128568-05-8 CAPLUS

CN Morpholine, 4-[[2-[(3,4-dichlorophenyl)amino]-4-(3,4-dimethoxyphenyl)-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 128568-06-9 CAPLUS

CN Morpholine, 4-[[2-[(4-bromo-2-chlorophenyl)amino]-4-(3,4-dimethoxyphenyl)-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 128568-07-0 CAPLUS

CN Morpholine, 4-[[2-[(3-chloro-4-fluorophenyl)amino]-4-(3,4-dimethoxyphenyl)-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

L4ANSWER 42 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

1986:186441 CAPLUS ΑN

104:186441 DN

ΤI Pharmaceutically useful pyrimidines

ΙN Hashimoto, Masashi; Robinson, David Hulme

PΑ Fisons PLC, UK

SO Eur. Pat. Appl., 42 pp.

CODEN: EPXXDW

DT Patent

LΑ English

F.

FAN.CNT 1							
	PATENT NO.	KIND	DATE	APPLICATION NO.	DÁTE		
		<del>-</del>	<b></b>				
ΡI	EP 164204	A1	19851211	EP 1985-302902	19850425		
	R: AT, BE, CH,	DE, FR,	, GB, IT, LI	, LU, NL, SE	,		
	DK 8502039	Α	19851113	DK 1985-2039	19850508		
	FI 8501837	A	19851113	FI 1985-1837	19850509		
	ZA 8503522	Α	19860326	ZA 1985-3522	19850509		
	NO 8501877	Α	19851113	NO 1985-1877	19850510		
	AU 8542276	A1	19851114	AU 1985-42276	19850510		
	JP 60246377	A2	19851206	JP 1985-98167	19850510		
	ES 543047	A1	19860716	ES 1985-543047	19850510		
	CN 85103378	Α	19860709	CN 1985-103378	19850514		
PRAI	GB 1984-12184	A	19840512				
	GB 1985-417	A	19850108				
	EP 1985-302902	Α	19850425	•			

OS MARPAT 104:186441

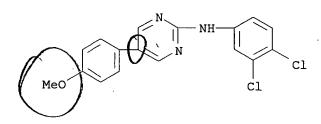
AΒ The title compds. [I; RR6 or R3R6 = bond; R = H, alkyl, aralkyl, Ph, alkanoyl; R1 = (un)substituted Ph, pyridinyl, pyrimidinyl, thiazolyl, pyrazinyl, pyridazinyl, imidazolyl; R2, R4, R5 = H, alkyl, alkoxy, OH, R1; R3 = H, alkyl, aralkyl, Ph; R2R4, R2R5 = CH:CHCH:CH] were prepared by cyclocondensation of RR1C(:NR3)NH2 (II) with ZR5C:CR2COR4 (III, Z =leaving group). Thus, 10.0 g II. (HO) 2CO (R = Ph, R1 = R3 = H) and 10.0 gIII (R2 = 4-MeOC6H4, R4 = R5 = H, Z = Me2N) were refluxed 17 h in pyridine to give 5.4 g pyrimidinamine IV. In mice I restore immune response depressed by presence of implanted Lewis lung sarcoma or by administration of cyclophosphamide.

ΙT 101987-04-6P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as immune adjuvant)

RN101987-04-6 CAPLUS

CN 2-Pyrimidinamine, N-(3,4-dichlorophenyl)-5-(4-methoxyphenyl)- (9CI) INDEX NAME)



ANSWER 43 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN1970:55485 CAPLUS

DN 72:55485

ΤI Antiinflammatory 2-anilino-5-methyl-6-phenylpyrimidines

Wagner, Hans A. IN

PA G.D. Searle and Co.

SO U.S., 3 pp. CODEN: USXXAM

יית Patent

LА English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3481932	Α	19691202	US 1967-664911	19670901
PRAI US 1967-664911	Α	19670901		

AΒ The title compds. (I) useful as antihypercholes-teremics, as antiprotozoal, and antiinflammatory agents, are prepared Thus, a mixture of 246 g 2-ethylthio-5-methyl-6-phenyl-4-pyrimidinol and 93 g PhNH2 in 1000 g Cellosolve was refluxed for 48 hr to give 2-anilino-5-methyl-6-phenyl-4pyrimidinol (II). A mixture of 15 g II and 70 g POC13 was refluxed 40 min to give 2-anilino-4-chloro-5-methyl-6-phenylpyrimidine. I (X = H, Z = C1)(III). A solution of 100 g III and 26 g NaN3 in 700 cc Me2CO was stirred 5  $\,$ hr at  $70-80^{\circ}$  to give I (X = H, Z = N3) (IV). A mixture of 1 g 5% Pd/C, 5 g IV and 100 g dioxane was stirred with H at 1 atm at room temp 18 hr to give I (X = H, Z = NH2). The following I were similarly prepared using a substituted aniline (X and Z, given): 2-F, Cl; 4-Cl, Cl (m. 183-4°); 4-Cl, N3 (m. 129-30°); 3-Br, Cl; 4-I, Cl; Cl, NH2 (m. 159-61°).

IT 26487-70-7P 26487-71-8P 26487-72-9P

> RL: IMF (Industrial manufacture); PREP (Preparation) (manufacture and pharmacological activity of)

RN26487-70-7 CAPLUS

CN Pyrimidine, 4-chloro-2-(p-chloroanilino)-5-methyl-6-phenyl- (8CI) (CA INDEX NAME)

2.6487-71-8 CAPLUS

CN Pyrimidine, 4-azido-2-(p-chloroanilino)-5-methyl-6-phenyl- (8CI) (CA INDEX NAME)

RN 26487-72-9 CAPLUS CN Pyrimidine, 4-amino-2-(p-chloroanilino)-5-methyl-6-phenyl- (8CI) (CA INDEX NAME)

L4 ANSWER 44 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1956:57198 CAPLUS

DN 50:57198

OREF 50:10801d-i

TI 4-Hydroxy-5-alkyl-6-phenylpyrimidine derivatives

IN Rorig, Kurt J.; Nicholson, Robert T.

PA G.D. Searle and Co.

DT Patent

LA Unavailable

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI US 2740785 19560403 US 1954-436992 19540615

AB 6,5,4,2-ArR''(HO)(RR'N)-tetrasubstd. pyrimidines where Ar is a lower aryl radical, R is a lower alkyl, aryl, haloaryl, or lower alkylcarbonyl radical, R' is H or a lower alkyl radical, and R'' is a lower alkyl were prepared The compds. are diuretics and bacteriostatic agents.
[H2NC(:NH)NH2].H2CO3 (I) (170), MeCHBzCO2Et (II) 325, and EtOH 1000 parts refluxed 12 h., then kept 24 h. at 0°, and the precipitate filtered off (the filtrate on concentration furnished addnl. material) afforded 2-amino-5-methyl-6-phenyl-4-pyrimidinol (III) (HCl salt, m. 225-7°). III 30 and fused NaOAc 60 ground to a fine powder, treated with Ac2O 195, the mixture stirred and refluxed 3 h., stirred with cold water 2000 parts, and the resulting precipitate filtered off and washed

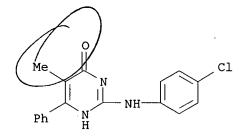
with

water gave the 2-AcHN analog, m. 289-90°. Similarly, from II, H2NCSNH2 (IV), Na, and EtOH was obtained the 2-HS analog of III, m. 236-7° (from dilute EtOH), which on alkylation (EtBr, Na, EtOH) gave the 2-EtS compound (V), m. 192-3°. V with Me2NH and EtOH heated 16  $\,$ h. at 150° in a rocking bomb gave the 2-Me2N analog of III, white needles, m. 258-9°. III refluxed with POC13 gave the 4-Cl compound (VI), prisms, m.  $131-2.5^{\circ}$  (from EtOH), which with alc. NaHS afforded the 4-HS compound (VII), m. 270-4  $^{\circ}$  (decomposition). VII with Ac2O and pyridine gave the 2-AcNH compound, m. 241-4°. I and BuCHBzCO2H yielded 2-amino-5-butyl-6-phenyl-4-pyrimidinol, m. 300-2° (decomposition), which after treatment with EtCO2Na and (EtCO)20 gave the 2-EtCONH analog, colorless, high-melting. 2,5-Me2C6H3CHMeCO2Et, IV, and Na in EtOH stirred and refluxed 8 h. furnished 2-mercapto-5-methyl-6-(2,5-dimethylphenyl)-4-pyrimidinol (VIII). VIII with EtBr, EtOH, and Na gave the 2-EtS compound which with Et2NH in EtOH after shaking in a bomb 16 h. at 150° afforded the 2-Et2N compound, white prisms, recrystd. from EtOCH2CH2OH (IX). V refluxed 50 h. with PhNH2 in IX gave the 2-PhNH compound, crystalline precipitate; 2-p-ClC6H4NH analog, m.

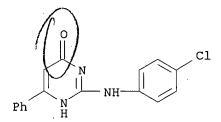
265-6.5° (with prior sintering at 260° (from EtOH)).

RN 500692-27-3 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[(4-chlorophenyl)amino]-5-methyl-6-phenyl- (9CI) (CA INDEX NAME)

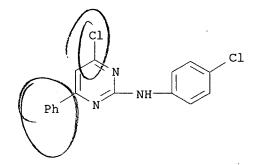


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ANSWER 45 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
AN
     1948:8848 CAPLUS
DN
     42:8848
OREF 42:1972c-f
     4-Hydroxypyrimidine derivatives
     Curd, Francis H. S.; Raison, Clifford G.; Rose, Francis L.
IN
PΑ
     Imperial Chemical Industries Ltd.
DT
     Patent
LΑ
     Unavailable
FAN.CNT 1
     PATENT NO.
                            KIND
                                    DATE
                                                 APPLICATION NO.
                                                                           DATE
     _____
     US 2433439
PΙ
                                    19471230
                                                 US
     The compds. are prepared by heating in EtOCH2CH2OH the appropriate arylamine
AΒ
     and a 4-hydroxypyrimidine substituted in the 6-position by a hydrocarbon
     radical and in the 2-position by an alkylmercapto or substituted
     alkylmercapto group. The preparation of the following 2-derivs. of
     4-hydroxy-6-methylpyrimidine is described: p-chloroanilino, colorless
     thick laminas, m. 294°; p-methoxyanilino, m. 212-13°;
     p-ethoxyanilino, m. 187-9°; p-bromoanilino, m. 284-6°; p-butylanilino, m. 195-6°; p-carbomethoxyanilino, m. 274-6°;
     p-phenyl-anilino, m. 258-9°; p-cyanoanilino, m. 330°;
     (2-naphthylamino), colorless needles, m. 243-5°; (1-naphthylamino),
     m. 256-7°; (4-chloro-1-naphthylamino), m. 298-301°
     (6-bromo-2-naphthylamino), colorless crystals, m. 286-8°;
     (6-methoxy-2-naphthylamino), colorless crystals, m. 238-9°;
     (2,4-dichloroanilino), m. 278-80°; (3,4-dichloroanilino), m. 250-2°; (2,5-dichloroanilino), m. 244-6°;
     (2-methyl-4-chloroanilino), m. 252-4°; (3-chloro-4-methylanilino), m. 252-4°; (3-chloroanilino), m. 227-9°; (2-chloroanilino), m. 244-6°; anilino, m. 244-6°; (3,4-dimethylanilino), m.
     238-9°; (3,5-dimethylanilino), m. 268°; (3,5-
     dibromoanilino), almost colorless needles, m. 325°;
     (2-methoxyanilino), colorless needles, m. 245-6°;
     (2-methylanilino), m. 204°; (3-methylanilino), m. 212-13°;
     (4-dimethyl-aminoanilino), m. 240-2°; p-toluidino, colorless
     crystals, m. 230°; (p-methylmercaptoanilino), m. 210-12°;
     p-nitroanilino, m. above 300°. 2-p-Ckloroanilino-4-hydroxy-6-
     phenylpyrimidine, colorless needles, m. 312-13°. Cf. C.A. 40,
     5054.6.
IT
     857413-75-3, 4-Pyrimidinol, 2-p-chloroanilino-6-phenyl-
         (preparation of)
RN
     857413-75-3 CAPLUS
CN
     4-Pyrimidinol, 2-p-chloroanilino-6-phenyl- (5CI) (CA INDEX NAME)
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ANSWER 46 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
     1948:8847 CAPLUS
ΑN
DN
     42:8847
OREF 42:1971h-i,1972a-c
     4-Halo-6-methylpyrimidine derivatives
IN
     Curd, Francis H. S.; Raison, Clifford G.; Rose, Francis L.
PA
     Imperial Chemical Industries Ltd.
DΤ
     Patent
LΑ
     Unavailable
FAN.CNT 1
     PATENT NO.
                                                                           DATE
                           KIND
                                   DATE
                                                 APPLICATION NO.
PΙ
     US 2433440
                                   19471230
                                                 US
     The compds. are prepared by heating a 4-hydroxy derivative of
6-methylpyrimidine
     (I), e.g. 2-p-chloroanilino-4-hydroxy-6-methylpyrimidine, and a
     halogenating agent, e.g. POCl3. The excess POCl3 is distilled in vacuo, ice
     and water are mixed in, then NH3 is added to faint alkalinity with stirring.
     The solidified product is crystallized from EtOH. The following 2-derivs. of
     4-chloro-6-methylpyrimidine are reported: p-chloroanilino, m.
     126-7°; p-methoxyanilino, m. 103-5°; (p-ethoxyphenyl), m.
     116-18°; p-toluidino, irregular colorless tabular crystals, m.
     104-6°; (p-methylmercaptoanilino), m. 81-2°; p-cyanoanilino, m. 215-16°; p-nitroanilino, m. 248-50°; (2-naphthylamino),
     colorless thick prisms, m. 145-7°; (6-bromo-2-naphthylamino),
     needles, m. 152-3°; (6-methoxy-2-naphthylamino), m. 148-50°;
      (2,4-dichloroanilino), m. 120-2°; (3,4-dichloroanilino), m.
     134-6°; (3,5-dibromoanilino), m. 131-2°;
      (2-methyl-4-chloroanilino), m. 107-8°; (3-chloro-4-methylanilino),
     m. 115-17°; (2,5-dichloroanilino), m. 101°;
     (3,4-dimethylanilino), m. 128-9^{\circ}; (3,5-dimethylanilino), m. 86-8^{\circ}; (4-bromoanilino), m. 140-1^{\circ}; (4-butylanilino), m.
     51-3°; (3-chloroanilino), m. 116-18°; (2-chloroanilino), m. 99-100°; (2-methylanilino), m. 116-18°; (3-methylanilino),
     m. 101-2°; anilino, colorless needles, m. 92-4°;
      (2-methoxyanilino), m. 103-4°; (4-dimethylaminoanilino), m.
     157-9°; (4-carbomethoxyanilino), m. 223-5°;
      (4-phenylanilino), m. 124-5°; (1-naphthylamino), m. 131-2°;
      (4-chloro-1-naphthylamino), m. 170°. 2-(4-Chloroanilino)-4-chloro-
      6-phenylpyrimidine m. 166-8°. Cf. C.A. 40, 5054.6.
IT
     859208-32-5, Pyrimidine, 4-chloro-2-p-chloroanilino-6-phenyl-
         (preparation of)
RN
     859208-32-5 CAPLUS
     Pyrimidine, 4-chloro-2-p-chloroanilino-6-phenyl- (5CI) (CA INDEX NAME)
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ANSWER 47 OF 47 CAPLUS COPYRIGHT 2006 ACS on STN
L4
AN
     1946:25718 CAPLUS
     40:25718
DN
OREF 40:5062a-i,5063a-f
     Synthetic antimalarials. VII. 2-Arylamino-4-dialkylaminoalkylaminopyrimidi
     nes. Variation of substituents in the 5- and the 6-position
ΑU
     Curd, F. H. S.; Richardson, D. N.; Rose, F. L.
CS
     Imperial Chem. Industries, Ltd., Manchester 9
     Journal of the Chemical Society (1946) 378-84
     CODEN: JCSOA9; ISSN: 0368-1769
     Journal
DT
LΑ
     Unavailable
AΒ
     The studies in Parts I and II have been extended to compds. having no
     substituent in the 6-position, a 6-Ph group, and various substituents in
     the 5-position (with and without a 6-Me group). An attempt has been made
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to increase their activity by the synthesis of structures capable not only of riboflavin antagonism but also, possibly, of interference with nucleoside synthesis on the basis of the hypothesis (Part III) that pyrimidine derivs. bearing a substituent in position 5 and an aminoalkylamino group in position 4 might be capable of functioning in this way. 2-p-Chloroanilino-4-hydroxypyrimidine, m. 242-4°, results in 21.5-g. yield from 18 g. 4-hydroxy-2-methylmercaptopyrimidine and 32 g. p-ClC6H4NH2 in 50 cc. EtOCH2CH2OH on refluxing 26 h.; 4-Cl derivative, m. 124°. 4-Hydroxy-2-methylmercapto-6-phenylpyrimidine (8.2 g.) and 12 g. p-ClC6H4NH2, heated 6 h. at 130-40 $^{\circ}$ , give 9.7 g. of 2-p-chloroanilino-4-hydroxy-6-phenylpyrimidine, m. 312-13°; 4-C1 derivative, m. 166-8°. 4-Hydroxy-2-(ethylmercapto)-5,6dimethylpyrimidine (15 g.) and 26 g. p-ClC6H4NH2, heated 9 h. at 130-40°, give 20.85 g. of 2-p-chloroanilino-4-hydroxy-5,6dimethylpyrimidine, m. 270-2°; 4-Cl derivative, m. 161-2°. 2-p-Chloroanilino-4-hydroxy-6-methyl-5-ethylpyrimidine, m. 246-7°; 4-Cl derivative, m. 128-30°. 2-p-Chloroanilino-4-hydroxy-5-benzyl-6-methylpyrimidine, m. 258-60°; 4-Cl derivative, m. 124-5°. 4-Hydroxy-2-methylmercapto-6-methylpyrimidine (45 g.) and Br in AcOH give 41 g. of the 5-Br derivative, m.  $254-6\degree$ ; 11.75 g. and 12.75 g. p-ClC6H4NH2 in 25 cc. EtOCH2CH2OH, heated at  $120-30^{\circ}$  for 26 h., give 11.75 g. of 5-bromo-2-p-chloroanilino-4-hydroxy-6-methylpyrimidine, m. 267-9° (decomposition); 4-Cl derivative, m. 176-8°. Et cyclohexanone-2-carboxylate (I) (29 g.) and 24 g. S-methylisothiourea sulfate in 150 cc. H2O containing 12 g. KOH, allowed to stand overnight, give 4.7 g. of 4-hydroxy-2-methylmercapto-5,6-cyclohexenopyrimidine (II), m. 220-2°. I (34 g.) and 16 g. CS(NH2)2, added to 12 g. Na in 300 cc. MeOH and the mixture refluxed 5.5 h., give 20.8 g. of 4-hydroxy-2-mercapto-5,6-cyclohexenopyrimidine, m. 314-20° (decomposition); 18.2 g. in 50 cc. 10% KOH, treated with 15 g. Me2SO4 in small portions, gives 11.15 g. of II. II (14.8 g.) and 24 g. p-ClC6H4NH2, heated 6 h. at 130-40°, give 19.4 g. of 2-p-chloroanilino-4-hydroxy-5,6-cyclohexenopyrimidine, m. 284-7°; 4-Cl derivative, m. 137-8°. 4-Hydroxy-2-methylmercapto-5,6-cyclopentenopyrimidine, m. 270-2°; 2-p-chloroanilino-4-hydroxy-5,6-cyclopentenopyrimidine, m. 244-6°; 4-Cl derivative, m. 151-2°. 2-p-Chloroanilino-4-hydroxy-5-methylpyrimidine, m. 266-7°; 4-Cl derivative, m. 158-9°. 2-p-Chloroanilino-4-hydroxy-5-phenylpyrimidine, m. 328-30°; 4-Cl derivative, m. 133-4°. 2-p-Anisidino-4-hydroxy-5-phenylpyrimidine, m. 271-2°; 4-Cl derivative, m. 152°. 2-p-Chloroanilino-4-hydroxy-5-phenoxypyrimidine, m. 240-2°; 4-Cl derivative, m. 112-13°. 2-p-Chloroanilino-4-(2diethylaminoethylamino)pyrimidine (III), m. 71-2°, active at 160°, inactive at 80 mg./kg. (di-HCl salt, with 1.5 mols. H2O, m.

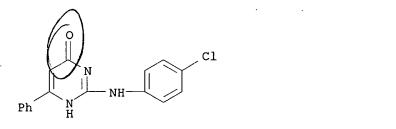
237-8°); 4-(3-diethylaminopropylamino) homolog, an oil, activity same as III; di-HCl salt, with 2 mols. H2O, m. 208-10°; dipicrate, m. 218-20°. 2-p-Chloroanilino-4-(2-diethylaminoethylamino)-6phenylpyrimidine, an oil, questionable activity at 160 mg./kg.; di-HCl salt, m. 277-9°. 2-p-Chloroanilino-4-(2-diethylaminoethylamino)-5,6-dimethylpyrimidine, m.  $100-2^{\circ}$ , active at 40 mg./kg.; di-HCl salt, with 1 mol. H2O, m.  $270-2^{\circ}$ ; 4-(3-diethylaminopropylamino)homolog, m. 104-6°, marked activity at 80 mg./kg.; di-HCl salt, with 1 mol. H2O, m. 277-9° (decomposition); 4-(3dimethylaminopropylamino) homolog, m. 116-18°, marked activity at 40 mg./kg.; di-HCl salt, with 1 mol. H2O, m. 238-40°. 2-p-Chloroan ilino-4-(2-diethylaminoethylamino)-5-ethyl-6-methylpyrimidine, m.  $92-4^{\circ}$ , active at 80 mg./kg.; di-HCl salt, with 0.5 mol. H2O, m. 258-60°; 4-(2-dimethylaminoethylamino) homolog, m. 115-16°, active at 80, inactive at 40 mg./kg.; di-HCl salt, with 1 mol. H2O, m. 262°; 4-(3-diethylaminopropylamino) homolog, m. 108-9°, active at 80, inactive at 40 mg./kg.; di-HCl salt, with 1 mol. H2O, m. 272-4°; 4-(3-dimethylaminopropylamino) homolog, m. 126-8°, marked activity at 80 mg./kg.; di-HCl salt, with 1.5 mols. H2O, m. 244-6°; 4-(4-diethylamino-1-methylbutylamino) homolog, an oil, active at 160, inactive at 120 mg./kg.; di-HCl salt, with 1.5 mols. H2O, m. 231-3°. 2-p-Chloroanilino-4-(2-diethylaminoethylamino)-5-benzyl-6-methylpyrimidine, m. 114-15°, active at 40 mg./kg.; di-HCl salt, with 0.5 mol. H2O, m. 255-6°; 4-(3-diethylaminopropylamino) homolog, m. 104-5°, active at 160, inactive at 80 mg./kg.; di-HCl salt, m. 274-6° (decomposition); 4-(3-dimethylaminopropylamino) homolog, m. 112-14°, active at 160 mg./kg.; di-HCl salt, with 1 mol. H2O, m.  $254-6^{\circ}$ ; 4-(4-diethylamino-1-methylbutylamino) homolog, an oil,  $\pm$ activity at 160 mg./kg.; di-HCl salt, with 0.5 mol. H2O, m.  $242-4^{\circ}$ . 2-p-Chloroanilino-4-(3-diethylaminopropylamino)-5-bromo-6methylpyrimidine, m. 94-6°, active at 400 mg./kg.; di-HCl salt, with 0.5 mol. H2O, m. 238-40°. 2-p-Chloroanilino-4-(2diethylaminoethylamino)-5,6-cyclohexenopyrimidine, m. 132-4°, marked activity at 200, active at 80, inactive at 40 mg./kg.; di-HCl salt, with 2 mols. H2O, m. 224-6°; 4-(3-diethylaminopropylamino) homolog, m. 138-40°, active at 40 mg./kg.; di-HCl salt, with 1.5 mols. H2O, m. 202-4°; 4-(3-dimethylaminopropylamino) homolog, m.  $125-7^{\circ}$ , active at 10 mg./kg.; di-HCl salt, m. 290° (decomposition). 2-p-Chloroanilino-4-(3-dimethylaminopropylamino)-5,6cyclopentenopyrimidine, m. 142-4°, active at 80 mg./kg. 2-p-Chloroanilino-4-(2-diethylaminoethylamino)-5-methylpyrimidine, m. 106-8°, inactive; di-HCl salt, m. 269° (decomposition). 2-p-Chloroanilino-4-(2-diethylaminoethylamino)-5-phenylpyrimidine, m. 152-3°, ± activity at 160 mg./kg.; di-HCl salt, m. 264-6°; 4-(3-diethylaminopropylamino) homolog, m. 155-6°, inactive; di-HCl salt, m. 264-6°. 2-p-Chloroanilino-4-(2diethylaminoethylamino)-5-phenoxypyrimidine, m. 84-5°, ± activity at 160 mg./kg. 2-p-Toluino-4-(2-diethylaminoethylamino) pyrimidine di-HCl, with 1 mol. H2O, m. 220-1°. 2-p-Anisidino-4-(2-diethylaminoethylamino)-5-phenylpyrimidine, m. 158-9°; di-HCl salt, with 1.5 mols. H2O, m. 209-11°. Full biol. details will be published and discussed elsewhere. 857413-75-3, 4-Pyrimidol, 2-(p-chloroanilino)-6-phenyl-858269-66-6, 4-Pyrimidol, 2-(p-chloroanilino)-5-phenyl-859208-32-5, Pyrimidine, 4-chloro-2-(p-chloroanilino)-6-phenyl-861032-41-9, Pyrimidine, 2-(p-chloroanilino)-4-(2diethylaminoethylamino)-6-phenyl-, dihydrochloride 861032-43-1, Pyrimidine, 2-(p-chloroanilino)-4-(2-diethylaminoethylamino)-6-phenyl-

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861032-45-3, Pyrimidine, 2-(p-chloroanilino)-4-(2-diethylaminoethylamino)-5-phenyl-, dihydrochloride 861032-47-5, Pyrimidine, 2-(p-chloroanilino)-4-(2-diethylaminoethylamino)-5-phenyl-861032-61-3, Pyrimidine, 2-(p-chloroanilino)-4-(3-diethylaminopropylamino)-5-phenyl-, dihydrochloride 861032-63-5, Pyrimidine, 2-(p-chloroanilino)-4-(3-diethylaminopropylamino)-5-phenyl-861032-86-2, Pyrimidine, 4-chloro-2-(p-chloroanilino)-5-phenyl-(preparation of)

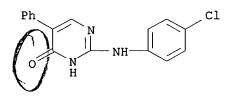
RN 857413-75-3 CAPLUS
CN 4-Pyrimidinol, 2-p-chlor

4-Pyrimidinol, 2-p-chloroanilino-6-phenyl- (5CI) (CA INDEX NAME)



RN 858269-66-6 CAPLUS

CN 4-Pyrimidol, 2-(p-chloroanilino)-5-phenyl- (4CI) (CA INDEX NAME)



RN 859208-32-5 CAPLUS

CN Pyrimidine, 4-chloro-2-p-chloroanilino-6-phenyl- (5CI) (CA INDEX NAME)

RN 861032-41-9 CAPLUS.

CN Pyrimidine, 2-(p-chloroanilino)-4-(2-diethylaminoethylamino)-6-phenyl-, dihydrochloride (4CI) (CA INDEX NAME)

## ●2 HCl

RN 861032-43-1 CAPLUS

CN Pyrimidine, 2-(p-chloroanilino)-4-(2-diethylaminoethylamino)-6-phenyl-(4CI) (CA INDEX NAME)

RN 861032-45-3 CAPLUS

CN Pyrimidine, 2-(p-chloroanilino)-4-(2-diethylaminoethylamino)-5-phenyl-, dihydrochloride (4CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{N} \\ \hline \text{Et}_2\text{N}-\text{CH}_2-\text{CH}_2-\text{NH} & \text{N} \end{array}$$

## ●2 HC1

RN 861032-47-5 CAPLUS

CN Pyrimidine, 2-(p-chloroanilino)-4-(2-diethylaminoethylamino)-5-phenyl-(4CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{N} \\ \hline \text{Et}_2\text{N}-\text{CH}_2-\text{CH}_2-\text{NH} & \text{N} \end{array}$$

RN 861032-61-3 CAPLUS

CN Pyrimidine, 2-(p-chloroanilino)-4-(3-diethylaminopropylamino)-5-phenyl-, dihydrochloride (4CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{N} \\ \hline \text{Et}_2\text{N}-\text{(CH}_2)_3-\text{NH} & \text{N} \\ \end{array}$$

## ●2 HCl

RN 861032-63-5 CAPLUS

CN Pyrimidine, 2-(p-chloroanilino)-4-(3-diethylaminopropylamino)-5-phenyl-(4CI) (CA INDEX NAME)

RN 861032-86-2 CAPLUS

CN Pyrimidine, 4-chloro-2-(p-chloroanilino)-5-phenyl- (4CI) (CA INDEX NAME)

=> => d his

(FILE 'HOME' ENTERED AT 17:10:41 ON 15 NOV 2006)

FILE 'REGISTRY' ENTERED AT 17:10:47 ON 15 NOV 2006

L1 STRUCTURE UPLOADED

L2 9 S L1 SSS SAM

L3 378 S L1 SSS FUL

FILE 'CAPLUS' ENTERED AT 17:14:01 ON 15 NOV 2006

L4 47 S L3

FILE 'CAOLD' ENTERED AT 17:15:02 ON 15 NOV 2006

=> s 13

L5 0 L3

=> log y

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION

FULL ESTIMATED COST 0.44 410.44

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE 0.00 -35.25

STN INTERNATIONAL LOGOFF AT 17:15:14 ON 15 NOV 2006